

Ambient Approximation of Functions and Functionals on Embedded Submanifolds



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Abstract of the Thesis

While many problems of approximation theory are already well-understood in Euclidean space and its subdomains, much less is known about problems on submanifolds of that space. And this knowledge is even more limited when the approximation problem presents certain difficulties like sparsity of data samples or noise on function evaluations, both of which can be handled successfully in Euclidean space by minimisers of certain energies. On the other hand, such energies give rise to a considerable amount of techniques for handling various other approximation problems, in particular certain partial differential equations.

The present thesis provides a deep going analysis of approximation results on submanifolds and approximate representation of intrinsic functionals: It provides a method to approximate a given function on a submanifold by suitable extension of this function into the ambient space followed by approximation of this extension on the ambient space and restriction of the approximant to the manifold, and it investigates further properties of this approximant. Moreover, a differential calculus for submanifolds via standard calculus on the ambient space is deduced from Riemannian geometry, and various energy functionals are presented and approximately handled by an approximate application of this calculus. This approximate handling of functionals is then employed in several penalty-based methods to solve problems such as interpolation in sparse data sites, smoothing and denoising of function values and approximate solution of certain partial differential equations.

German Summary — Deutsche Zusammenfassung

Die vorliegende Dissertationsschrift befasst sich mit Problemen der Approximation auf eingebetteten Untermannigfaltigkeiten des euklidischen Raumes.

Nach einer kurzen Einführung über geeignete Untermannigfaltigkeiten und über Funktionenräume auf ebensolchen erweitert sie zunächst bekannte Konvergenzresultate für die sogenannte *ambient approximation method* und deren bisher wichtigsten Spezialfall, die *ambient B-spline method*. Insbesondere generalisiert sie diese auf Untermannigfaltigkeiten mit höherer Codimension und ergänzt die betreffenden Resultate um Ergebnisse zu Approximation unter einer endlichen, festen Anzahl an Interpolationsbedingungen und um Approximationsaussagen zur Ableitung entlang des Normalenbündels der Untermannigfaltigkeit.

Im Anschluss wird ein intrinsischer, tangentialer Calculus für solche Untermannigfaltigkeiten eingeführt, der auf bestehenden Konzepten der riemannschen Geometrie basiert. Dabei wird insbesondere die Beziehung zwischen intrinsischer, tangentialer Ableitung und der korrespondierenden euklidischen Ableitung entlang von Elementen des Tangentialraums beleuchtet. Außerdem werden in diesem Zusammenhang eine Reihe von intrinsischen Funktionalen eingeführt, und es wird insbesondere das Konzept der polynomiellen Unisolvenz in die Situation des tangentialen Calculus übertragen.

Als nächstes wird eine Methodik vorgestellt, die die Approximation der Optima besagter Funktionele mittels im Kern extrinsischer Methoden erlaubt, die sich auf die sogenannten *penalty*-Verfahren beziehen. Für die resultierende *ambient penalty approximation* werden Konvergenzresultate präsentiert, und es werden beispielhaft verschiedene interessante Funktionele diskutiert, die unter anderem Extrapolation aus wenigen verstreuten Datenpunkten auf der Untermannigfaltigkeit M , Glättung von Funktionswerten über M und die näherungsweise Lösung elliptischer partieller Differentialgleichungen auf M erlauben.

Chapter 1

Introduction and Related Work

The problem of approximation of functions on manifolds, particularly surfaces, has gained both relevance and attraction over the last years. The relevance came with the increased capability and popularity of computer systems in representation, processing and simulation of problems in engineering, manufacturing and the natural and medical sciences. *Computer graphics* (CG), *medical imaging*, *computer aided design* (CAD) and *manufacturing* (CAM) or recently *industry 4.0* are just some of the keywords that one frequently encounters in this area. And the problems that need to be solved are as diverse as

- simulation of biological, physical or manufacturing processes on computer models, for example in terms of distributions of heat or material, deformation of models or calibration and registration between different states of one model during a manufacturing process,
- reasonable extrapolation of data measurements on real world surfaces from a comparably sparse set of data sites to the whole surface,
- high-detail approximation and processing of dense measurements on real world surfaces, including data reduction and the elimination of noise and measurement errors,
- reduction of data measurements for fast evaluation, compression and easy processing,
- and many more.

In mathematical terms, these lead to problems of approximation theory as diverse as *scattered data approximation*, *sparse data extrapolation*, *smoothing* and *noise reduction* and the solution of *partial differential equations* (PDE). Within this thesis, we are going to address all of these problems by essentially novel approaches to obtain approximate solutions.

Related Work

The problem of approximating a function $f : M \rightarrow \mathbb{R}$ for a given embedded submanifold M is quite a delicate matter even if the function is explicitly known or sampled in a very dense set of data sites $\Xi \subseteq M$ without any measurement errors. It has thus attracted numerous researchers over the past decades. Effectively, three types of approaches seem to exist:

The first approach is to parameterise the submanifold suitably by a finite number of parameter spaces with corresponding parameterisations and to solve the approximation problem on each parameter space independently before blending the local solutions with the help of the parameterisations. This approach was for example followed in [25, 26, 30, 31]: The authors use projections on the tangent plane of a submanifold to solve the approximation problem locally.

The second approach is to provide some set of truly intrinsic functions like *spherical harmonics* [8], *spherical splines* [10, 47], other functions on the sphere [86, 101, 104] or on more general manifolds [56]. Many of these are tailored for the sphere and thereby already illustrate the problem of this approach: for an arbitrary submanifold it can be quite complicated. Actually, the determination of suitable intrinsic functions can be a very difficult task in its own right — it may even be as complex as, or even more complex than, the given approximation problem; the authors of [43] provide a kind of hybrid of the first two approaches and employ a projection onto the sphere where the approximation problem is solved afterwards. So it is applicable only to sphere-like surfaces and effectively uses the sphere as its "chart". Similarly restricted to sphere-like surfaces are for example methods proposed in [4, 5, 91].

The third approach is to solve the approximation problem in the ambient space of the submanifold M and to restrict the solution to M afterwards. Such a method will benefit from the fact that there is often a well understood theory for approximation methods in Euclidean spaces, for example all kinds of splines, polynomials, kernel functions and the like: In particular, important properties like smoothness can be deduced directly from the corresponding properties in the ambient space; for radial basis functions (RBFs), this approach was recently investigated in [49], where the authors made also use of the fact that the restriction of such a kernel function is an intrinsic kernel as well. They found that for many kernels, this approach gave the same convergence behaviour as the corresponding kernel in a Euclidean space of the same dimension as that of the submanifold.

For tensor product splines and other methods that meet certain locality requirements, this approach was also investigated recently for the important case of hypersurfaces in [74, 75, 76, 82], where the authors proved that the approximation

order achievable in the ambient space is essentially reproduced by the restrictions — at least under some mild further restriction of the applicable norms. This approach will play a major role in the present thesis as well; it is based on extending an intrinsic function constantly along the normals of the submanifold, followed by application of the respective approximation method to this extension on the ambient space and restriction of the approximation to the submanifold.

While the problem of suitable approximation to function values in scattered data sites on submanifolds itself is a nontrivial issue even if the data is sufficiently dense, it can nonetheless be solved satisfactorily by some of the above approaches. But the problem becomes even more involved when the data is sparse. In fact, the literature on that matter is quite sparse itself. Of course, for the Euclidean situation, there exist well understood approaches that provide pleasant results: One are *polyharmonic splines* with the particular examples of *thin-plate splines* in \mathbb{R}^2 and *cubic splines* in \mathbb{R}^1 , see for example [17, 40, 105]. These minimise certain energies under fixed interpolation constraints in a finite set of points and can also be considered to be special cases of RBF. Other examples include *inverse distance weighting* [46, 53, 70, 48, 92, 105], sometimes also called *Shepard's method*, and *Kriging* [94]. Of course, these methods can be employed in the ambient space, just ignoring the geometry of the submanifold, and the solution on the submanifold would then be obtained by simple restriction. This can yield reasonable results if the geometry of the submanifold is very nice, for example a sphere, but as soon as the geometry is more intricate, significant artifacts will appear — we will present examples of this problem later in this thesis.

Considering the other approaches to approximation on submanifolds in general, we first see that any application of a method based on charts is effectively pointless in this setting: one could easily end up with parameter spaces that contain no data sites at all. On the other hand, the Euclidean approaches are essentially transferable to a purely intrinsic setting, particularly for the case of the sphere (cf. [58, 86, 104, 101]), but also for other specific (cf. [62]) and even more general manifolds (cf. [60, 59, 61]), like submanifolds that are compact and have no boundary. Further options include the spherical splines and spherical harmonics mentioned before. However, the case of more general manifolds often includes the solution of certain differential equations in that manifold. This means that first and foremost this submanifold needs to be known explicitly, not just by some discretisation, and can be a very challenging task for arbitrary manifolds. Moreover, the evaluation of these functions can be very costly: For example, even something as simple as a direct generalisation of the inverse distance weighting approach would require the calculation of n geodesic distances for n data sites in each evaluation. This can be quite significant if geodesic distances do not have a closed form expression like

in the spherical case, even if the nontrivial issue of existence of geodesics is solved at a satisfactory level. And for some of the other approaches mentioned above, there do not even exist closed form expressions for suitable functions on general manifolds, as the involved equations are by far too complex.

In the Euclidean case, the problem of smooth extrapolation often leads to corresponding solutions for problems of smoothing of (possibly noisy or oversampled) data: In the univariate case, the *smoothing splines* (cf. [33]) appear as generalisations of interpolating cubic splines, and for the multivariate setting smoothing problems are often addressed by methods that have a counterpart in extrapolation as well (cf. [33, 40, 48]). Consequently, the same holds also for the sphere (cf. [33, 101]) and presumably also for other manifolds. But with these approaches, the drawbacks of the corresponding extrapolation methods will of course remain present as well.

Finally, the solution of intrinsic partial differential equations for a given submanifold has also gained increased attraction in recent years and decades. Several approaches exist in the literature: The first is based on fairly obvious generalisations of standard methods in the Euclidean setting to the situation of an embedded submanifold, particularly *finite elements* over a suitable triangulation of the submanifold (cf. e.g. [35, 36]). However, this approach has the significant drawback that the discretisation of the submanifold is either very coarse — and in this case only a rough approximation of the actual surface — or the appearing linear systems are, though sparse, very large. And further, the quantities of the equation need to be discretised appropriately, which is a possibly nontrivial task in its own right — although for common operators there are suitable discretisations, cf. e.g. [36, 103].

The second approach is based on the idea that models, often stemming from CAD or CG, and spaces or sets of functions used for their parameterisations can be employed in the solution of the PDE. It firms under the name *isogeometric analysis*, cf. [11, 28] and is consequently a representative of the parametric approximation approach family: It exploits the presence of exact parameterisations for many CAD and CG models and uses a suitable *Galerkin formulation* based on the space or set of functions that is also employed in the parameterisation, typically tensor products of B-splines or NURBS. But as a direct consequence, this method is limited to these specific representations. Nonetheless, the approach has applications for problems both on submanifolds and in various domains of Euclidean space, and an overview of some approaches and applications is given in [22].

A third approach is based on so-called *collocation*, where the respective differential equation is solved for a finite but sufficiently dense set of points in the respective domain or submanifold, called *collocation points*, cf. [38, 39, 45]. This approach

has been transferred to the sphere [72]. The concept is further adapted in [50] for application on general surfaces by suitable discretisation of intrinsic differential operators, which can otherwise be hard to handle on arbitrary surfaces. In contrast to this, [84] approaches the intrinsic operators by enforcing certain constraints on the functions in collocation points in terms of normal derivatives that are familiar to the constraints occurring in this thesis.

Ultimately, a fourth approach involves the extension of the intrinsic equation into the ambient space, thereby introducing a new problem in the ambient space whose restriction solves the intrinsic problem. Methods of this kind are often based on a representation of the submanifold by an implicit function (cf. [15, 21, 27, 36, 54, 82]). Unfortunately, the extension introduces new difficulties: In particular, the problem may lose important properties like ellipticity (e.g. [36]) or introduce discontinuities (cf. [15]), and the extended domain introduces further boundaries for which appropriate boundary conditions may be required or have to be circumvented (cf. e.g. [15, 82]). Furthermore, essentially any of these methods is presented only for hypersurfaces.

In this thesis, we present approaches to the problems stated above that are capable of overcoming many of the issues and difficulties stated so far.

Outline of the Thesis

This thesis is organised as follows: In the following second chapter, we will introduce some basic facts and concepts for the treatment of embedded submanifolds within their ambient space. This includes in particular a method to extend functions defined on the submanifold into this ambient space. And we will also briefly revise and enhance certain facts about function spaces, particularly Sobolev spaces, for the treatment of functions on submanifolds.

The third chapter features results of approximation theory for submanifolds: We will generalise ideas from [74, 75, 76, 82] in various ways, particularly to a setting with codimension greater than one. There, we are able to deduce that under mild restrictions on the applicable norms we will be able to reproduce the rates of convergence available in the ambient space for approximations on submanifolds. These can be based on tensor product B-splines or other approximation methods that meet certain locality requirements. The general framework we propose, featured for codimension one in [76] as the *ambient approximation method* (AAM) and in [74, 82] for tensor product splines as the *ambient B-spline method* (ABM), is essentially applicable to any kind of embedded submanifold and easily implemented in practice.

Further, we will investigate certain other properties of this and related approaches in terms of achievable rates of convergence. In particular, we will find conditions under which the rate of convergence provided by tensor product splines is maintained under a finite, fixed set of interpolation constraints. And we will investigate rates of convergence that can be obtained simultaneously for the derivative along the *normals* of the submanifold, so an essentially extrinsic property. In the end, we support our results on the convergence order in the intrinsic setting with numerical examples, in particular for a surface embedded in \mathbb{R}^4 .

The fourth chapter introduces an intrinsic calculus for functions defined on submanifolds and its relation to the calculus of functions in the ambient space that yield intrinsic functions by restriction. This calculus is to some degree a degeneration of concepts from Riemannian geometry. In this, we are particularly interested in intrinsic versions of first and second order derivatives to a sufficiently (weakly) differentiable function f on an submanifold and their relation to extrinsic derivatives of a function F on the ambient space such that f is the restriction of F to the submanifold. We will find that the first order derivative of F along the normals of the submanifold plays a crucial role therein.

Further, we will introduce certain intrinsic functionals on submanifolds and investigate their properties. In particular, we will be interested in finding conditions under which a finite set Ξ of points yields that any function with vanishing intrinsic second order derivative that vanishes in these points must vanish itself. Thereby we transfer the concept of polynomial *unisolvency* on Euclidean space to the intrinsic setting. And we will introduce a couple of model functionals that will in the end lead to solutions for problems as diverse as the "optimal" extrapolation from sparse data, noise reduction, smoothing and the solution of certain *elliptic PDE*.

Chapter five introduces a general framework for the formulation and approximate solution of minimisation problems for the intrinsic functionals introduced in the third chapter. We will present a penalty-based minimisation approach called *ambient penalty approximation* (APA) that is capable of handling various functionals; in particular we can thereby treat the specific functionals we have introduced in the previous chapter for extrapolation from sparse data, noise reduction and the solution of elliptic PDE. We are able to present upper bounds on the convergence rate in the intrinsic energy norm induced by those functionals, which are at least in some cases optimal.

Chapter six applies the concepts of the fifth chapter to problems of extrapolation, smoothing and noise reduction. We will apply the results of chapter three to obtain theoretical rates of convergence and find that in fact the results are even better than the theory implies. Also, we present various numerical examples for both curves in \mathbb{R}^2 and surfaces in \mathbb{R}^3 that verify the validity of our method. And we will

additionally present a two-stage approximation method in terms of *radial basis functions* (RBF) and tensor product splines for scattered data problems that is afterwards integrated into a bilevel algorithm to solve scattered data problems with irregular samplings.

Finally, chapter seven presents the application of the results of chapter five to the partial differential "model" equation

$$\Delta_M f - \lambda f = g$$

for scalar $\lambda \geq 0$ and intrinsic Laplacian Δ_M of submanifold M . By various numerical examples we verify that the optimal convergence rate on compact submanifolds without boundary in the energy norm which chapter five has implied is indeed achievable. And we also provide examples for submanifolds with boundary, where the same approach under suitable boundary conditions leads to pleasant approximations of the solution with optimal convergence of the residual $\Delta_M f - \lambda f - g$.

We conclude our argumentation in chapter eight by summing up our main results, and we also discuss open problems and possible further developments there. Ultimately, a subsequent appendix features auxiliary statements and proofs left out in the main part of the thesis.

Chapter 2

Embedded Submanifolds and Function Spaces

In this chapter, we will give a basic introduction of what kind of embedded submanifolds we are going to work with. And we also give some brief introduction into basics of the theory we need for them. In addition, we will present a way to parameterise both the submanifold and its ambient space simultaneously. By this, we will be able to define extension operators for functions given only on the submanifold. In particular, we will encounter the *normal extension operator* that extends constantly along the normals of hypersurfaces, and constant in the normal space of submanifolds of higher codimension.

Further, we will briefly introduce and revise some important aspects of function spaces both in Euclidean space and on submanifolds, particularly Sobolev spaces. Most proofs and additional results are postponed to the appendix; we restrict ourselves here to the most important results that are frequently referred to in the thesis.

2.1 Embedded Submanifolds

In this section, we will introduce what types of embedded submanifolds we are going to deal with, and we will introduce the beforementioned extension operators. We will first clarify the concepts for compact submanifolds without boundary and the normal extension operator before we generalise the ideas to certain subdomains of such compact submanifolds and also to more general extension operators.

2.1.1 Closed Submanifolds, Normal Foliation and Normal Extension

We will be developing approximation concepts on embedded submanifolds (*ESMs*) later in this thesis, so we first have to make some introductory considerations about these structures. In particular, we need some basic definitions and certain important properties. Within this subsection, we are going to introduce or revise a collection of relevant properties for submanifolds that are compact, so they are closed, bounded and have no boundary. Standard examples of these include in particular the sphere and the torus. Certain embedded submanifolds with boundary will be treated later due to their increased complexity, once we have clarified our main ideas in the simpler case of a compact submanifold. In any case, we presume that our submanifold M is embedded into some \mathbb{R}^d , has dimension $k \in \{1, \dots, d-1\}$ and codimension $\kappa = d - k$.

2.1 Notation A smooth embedded submanifold M of \mathbb{R}^d of dimension k , compact and without boundary, is denoted by $M \in \mathbb{M}_{\text{cp}}^k(\mathbb{R}^d)$. More generally speaking, a smooth embedded submanifold M , compact and without boundary, of a smooth embedded submanifold \widehat{M} is denoted by $M \in \mathbb{M}_{\text{cp}}^k(\widehat{M})$.

Before we come to the specific properties we demand for our embedded submanifolds, we will have to introduce some basic concepts: The first is a suitable version of the well-known concept of a *bounded (strong) Lipschitz domain* (cf. [1, 2, 64, 100]) that we will restrict ourselves to. If we follow [2], this type of domain is given by demanding that there is a finite open cover $\{\Theta_j\}_{j \in J}$ of the compact boundary $\partial\Omega$ such that $\partial\Omega \cap \Theta_j$ is graph of a Lipschitz function for each $j \in J$.

We will use this kind of Lipschitz domains when Sobolev spaces are concerned. Therefore, they will soon be particularly important as *parameter spaces* of our submanifolds in order to define Sobolev spaces on submanifolds. In the remaining course of this thesis, we will use the following notation:

2.2 Notation If Ω is a bounded Lipschitz domain in \mathbb{R}^d , this is denoted by $\Omega \in \text{Lip}_d$. We also use the notation $\Omega \in \text{Lip}_d^*$ to express that either $\Omega \in \text{Lip}_d$ or $\Omega = \mathbb{R}^d$.

Most importantly, any Euclidean ball $B_r^d(x) := \{y \in \mathbb{R}^d : \|x - y\|_2 < r\}$ of fixed radius r is such a bounded (strong) Lipschitz domain, any maximum norm ball $B_r^d[x] := \{y \in \mathbb{R}^d : \|x - y\|_\infty < r\}$, so any hypercube, is such a bounded (strong) Lipschitz domain and any Cartesian product of the form $B_{r_1}^k(x_1) \times B_{r_2}^k[x_2]$ is also a bounded (strong) Lipschitz domain.

The second concept is a useful concept of boundedness of (diffeomorphic) maps, namely the concept of *C-boundedness*:

2.3 Definition

1. A smooth map $\varphi \in C^\infty(\Omega, \mathbb{R})$ on open domain $\Omega \subseteq \mathbb{R}^d$ is said to be *C-bounded* if for each $n \in \mathbb{N}_0$ there is a constant c_n such that any partial derivative of φ up to total order n is bounded by c_n on Ω .
2. If $\varphi : \Omega \rightarrow \mathbb{R}^d$ is a diffeomorphism, then it is said to be a *bidirectionally C-bounded diffeomorphism* if both φ and φ^{-1} are C-bounded maps.

Particularly important is that C-bounded diffeomorphisms preserve Lipschitz domains. That is, it holds the following proposition of [64]:

2.4 Proposition *If $\varphi : U \rightarrow \widehat{U}$ is a C-bounded smooth diffeomorphism and $\Omega \in \text{Lip}_d$ with $\text{clos}(\Omega) \subseteq U$, then $\varphi(\Omega) \in \text{Lip}_d$.*

Now we come to the additional assumptions for compact embedded submanifolds we will make. Namely, we will demand that the embedded submanifold is smoothly parameterised in a suitable way. So we presume that the ESM is equipped with a *finite* inverse atlas $\mathbb{A}_M = (\psi_i, \omega_i)_{i \in I}$ providing parameterisations ψ_i and parameter spaces ω_i such that it holds for any $i \in I$:

- $\omega_i \in \text{Lip}_k$ and there is superset $\omega_i^* \in \text{Lip}_k$ of ω_i such that $\text{clos}(\omega_i) \subseteq \omega_i^*$ and $\psi_i : \omega_i^* \rightarrow M$ is well-defined and injective on ω_i^* .
- There is a smooth map T^i that maps each $x \in \omega_i$ to an orthonormalised tangent frame (τ^1, \dots, τ^k) of M in $\psi_i(x)$.
- There is a smooth map N^i that maps each $x \in \omega_i$ to an orthonormalised normal frame (ν^1, \dots, ν^k) of M in $\psi_i(x)$.

2.5 Notation Any inverse atlas \mathbb{A}_M of an embedded submanifold M that meets these requirements is denoted by $\mathbb{A}_M \in \Pi(M)$.

2.6 Remark: In the following, we will identify $T^i(x)$ with $T^i(\psi_i(x))$ and $N^i(x)$ with $N^i(\psi_i(x))$. Furthermore, we will frequently omit the index "*i*" in T^i or N^i . We can do so because we will usually be either within a fixed parameter space of an inverse atlas as introduced above or in a situation where the quantities depending on T^i, N^i turn out to be invariant under rotations.

2.7 Important: By arguments provided in Section 9.1.2 of the appendix, we can choose any ω_i or ω_i^* as a ball or a cylinder of fixed height and radius, so

$$\begin{aligned} \omega_i &= B_\rho^k(0) & \text{or} & & \omega_i &= B_\rho^{k-1}(0) \times]-\rho, \rho[\\ \omega_i^* &= B_{\rho^*}^k(0) & \text{or} & & \omega_i^* &= B_{\rho^*}^{k-1}(0) \times]-\rho^*, \rho^*[\end{aligned}$$

with $\rho^* > \rho > 0$. This gives us C-boundedness of ψ_i, T^i, N^i on ω_i directly by compactness. For the rest of this thesis, we will presume to be equipped with an inverse atlas that meets these requirements.

As we are investigating ESMs in \mathbb{R}^d , the portion of the ambient space near an ESM will play a crucial role for us. More specifically, we will be particularly interested in sufficiently narrow *tubular neighbourhoods*:

2.8 Definition Let $M \in \mathbb{M}_{\text{cp}}^k(\mathbb{R}^d)$ and $x \in M$. We define the set $B_\rho^N(x)$ for $\rho > 0$ and $N_x M$ the *normal space* to M in $x \in M$ as

$$B_\rho^N(x) := B_\rho^d(x) \cap N_x M.$$

The union of all $B_\rho^N(x)$ of fixed radius ρ is called the *tubular neighbourhood* of M and denoted by $U_\rho(M)$. It is said to have the *closest point property* if any element $z \in U_\rho(M)$ has a uniquely determined closest point on M .

This definition leads us directly to the following proposition of [44]:

2.9 Proposition — Tubular Neighbourhood Theorem —

If $M \in \mathbb{M}_{\text{cp}}^k(\mathbb{R}^d)$, then there is a fixed $\varepsilon > 0$ such that $B_\varepsilon^N(x)$ and $B_\varepsilon^N(z)$ are disjoint for any $x \neq z \in M$. Consequently, $U_\varepsilon(M)$ has the closest point property. Further, the projection Π_M onto M defined for any $z \in U_\varepsilon(M)$ by

$$\Pi_M(z) = \arg \min_{x \in M} \|x - z\|_2.$$

is smooth in $U_\varepsilon(M)$.

Now we make some further considerations on the ambient space in which our ESM is embedded, and some considerations on normal maps. In later chapters, we will be interested in extending functions defined only on the ESM into the ambient space. So we would prefer to transfer as many intrinsic properties of this function into the extrinsic setting as possible. Our objective will then be to reduce an intrinsic version of the calculus on an ESM to some slightly adapted Euclidean calculus in the ambient space. And as a consequence of this, we will be able to deduce numerous other features.

We will see that a very good choice for this step from the ESM into the ambient space is an extension that is constant in the normal space. This can be accomplished by performing $f \circ \Pi_M$ for given $f : M \rightarrow \mathbb{R}$ and the orthogonal projection Π_M onto M . While this is already well defined by the existence and sufficient smoothness of the projection implied by [44] in a sufficiently narrow tubular neighbourhood, we will have to create a slightly more elaborate framework for our theoretical treatment of the problem in some contexts. In particular, we will create a suitable link from the ambient space to the specific inverse atlas we have just introduced.

We presume from now on that $\varepsilon > 0$ is so small that the tubular neighbourhood $U_\varepsilon(M)$ has the closest point property and choose an inverse atlas $\mathbb{A}_M = (\psi_i, \omega_i)_{i \in I} \in \mathbb{I}(M)$ for the ESM $M \in \mathbb{M}_{\text{cp}}^k(\mathbb{R}^d)$. Then we choose the set $\Omega_i^\varepsilon := \omega_i \times B_\varepsilon^k(0)$ and define

$$\Psi_i(x, z_1, \dots, z_K) := \psi_i(x) + \sum_{j=1}^K z_j \nu^j(x)$$

for the j -th normal $\nu^j(x)$ of normal frame $N^i(x)$. The resulting function has then a functional determinant with maximal rank and is thus a diffeomorphism that parameterises the tubular neighbourhood $U_\varepsilon(\psi_i(\omega_i))$. Moreover, we can deduce directly that for a suitable choice of ε this diffeomorphism is bidirectionally C -bounded: By our requirements on $(\psi_i, \omega_i) \in \mathbb{A}_M$ and the superset ω_i^* of ω_i we can see that Ψ_i is smooth and diffeomorphic on $\omega_i^* \times B_\delta^K(0)$ for sufficiently small $\delta > \varepsilon$. Thereby its restriction to $\omega_i \times B_\varepsilon^K(0)$ is obviously a bidirectionally C -bounded diffeomorphism there. We obtain the following conclusion:

2.10 Conclusion For any $M \in \mathbb{M}_{\text{cp}}^k(\mathbb{R}^d)$ and any sufficiently small $\varepsilon > 0$, there is an *extended inverse atlas* $\mathbb{U}_M^\varepsilon = (\Psi_i, \omega_i \times B_\varepsilon^K(0))_{i \in I}$ of $U_\varepsilon(M)$ such that each Ψ_i is a bidirectionally C -bounded diffeomorphism. Moreover, any $N_\xi^\varepsilon := \Psi_i(x \times B_\varepsilon^K(0))$ for $x \in \omega_i$ and $\xi = \psi_i(x)$ is a normal space ball $B_\varepsilon^N(\psi_i(x))$.

2.11 Remark: For any $i \in I$, the family of these balls $\{N_{\psi_i(x)}^\varepsilon\}_{x \in \omega_i}$ forms a so-called *foliation*⁽¹⁾ of $U_\varepsilon(\psi_i(\omega_i))$. Consequently, by considering all pairs of the inverse atlas we obtain a foliation of $U_\varepsilon(M)$ that we call the *normal foliation* \mathbb{F}_N . Therein, each normal space ball $N_\xi^\varepsilon = B_\varepsilon^N(\xi)$ for $\xi \in M$ is called a *leaf* of the foliation.

2.12 Remark: (1) A direct consequence of the smoothness of M and Prop. 2.4 is that $\Psi_i(\Omega_i^\varepsilon) \in \text{Lip}_d$ for each $i \in I$, and obviously $U_\varepsilon(M) \in \text{Lip}_d$ for sufficiently small $\varepsilon > 0$.

(2) In the following, we will simply write $U(M)$ and extended inverse atlas $\mathbb{U}_M = (\Psi_i, \Omega_i)_{i \in I}$ whenever the exact extent ε does not matter, provided it is sufficiently small and fixed.

(3) Note in particular that the foliation does not depend on the orientation of the normal frame. Consequently, any local rotation or even reflection of this does not modify the foliation. Thereby, it will also be well-defined for nonorientable surfaces like a Möbius strip.

2.13 Notation Any extended inverse atlas $\mathbb{U}_M = (\Psi_i, \Omega_i)_{i \in I}$ that satisfies the stated requirements and is determined by $\varepsilon > 0$ small enough that Conclusion 2.10 applies, is denoted by $\mathbb{U}_M \in \mathbb{II}_N^{\text{ex}}(M)$.

As we have already mentioned before, we have a well-defined projection which is smooth on any such tubular neighbourhood that is sufficiently narrow. Consequently, we can use this projection $\Pi_M : U(M) \rightarrow M$ to define an extension of functions on M into $U(M)$:

⁽¹⁾We will not require anything of the profound theory on foliations of Riemannian manifolds here, we just borrow the name from there. The interested reader is referred to [95].

2.14 Definition For any $M \in \mathbb{M}_{\text{cp}}^k(\mathbb{R}^d)$, the operation $E_N : f \mapsto f \circ \Pi_M$ determines an extension of a function $f \in C(M, \mathbb{R})$ into a sufficiently narrow tubular neighbourhood $U_\varepsilon(M)$. This extension is then called the *normal extension*. We will also denote $E_N f$ simply by \vec{F} .

2.15 Remark: (1) The regularity and smoothness of \vec{F} is guarded by the regularity and smoothness of f and Π_M .

(2) The function \vec{F} is constant on each leaf of F_N by construction. Consequently, if $N_\xi^\varepsilon = B_\varepsilon^N(\xi)$ is the leaf of F_N to $\xi \in M$ and thus an embedded submanifold of dimension κ in its own right, the directional derivative of $E_N f$ at any $x \in N_\xi^\varepsilon$ along any $\nu \in T_x N_\xi^\varepsilon$ must vanish. This is a consequence of the chain rule and the fact that $D_\nu \Pi_M$ vanishes there by definition. More specifically, we have for any $x, z \in N_\xi^\varepsilon$

$$\Pi_M(z) - \Pi_M(x) = 0.$$

By the smoothness of the leaf N_ξ^ε , this remains valid under taking limits of differential quotients.

(3) As the foliation, the extension is independent of the orientation of the normal frame. In particular, its smoothness does not depend on the transition between local choices of the normal frames.

A further direct consequence of our recent considerations is the local existence of normal frames for our ESMs that are locally smooth *in the neighbourhood* as well, which is the purpose of the next lemma. This fact will later be used to define a form of differential calculus intrinsic to an ESM:

2.16 Lemma Let $M \in \mathbb{M}_{\text{cp}}^k(\mathbb{R}^d)$ and let $U_M^\varepsilon = (\Psi_i, \omega_i \times B_\varepsilon^k(0))_{i \in I} \in \mathbb{I}_N^{\text{ex}}(M)$. Then for any sufficiently small $\varepsilon > 0$, any $i \in I$ and any $z \in \Psi_i(\omega_i \times B_\varepsilon^k(0))$ the maps

$$z \mapsto N^i(\Pi_M(z)), \quad z \mapsto T^i(\Pi_M(z))$$

are C -bounded on each $\Psi(\omega_i \times B_\varepsilon^k(0))$.

Proof: As we can demand that the map $z \mapsto N^i(\Pi_M(z))$ is well-defined and smooth even on $\Psi_i(\omega_i^* \times B_\delta^k(0))$ with sufficiently small $\delta > \varepsilon$, this is a direct consequence of compact containment $\Psi_i(\omega_i \times B_\varepsilon^k(0)) \Subset \Psi_i(\omega_i^* \times B_\delta^k(0))^{(2)}$. The same arguments apply to the tangent frame. \square

2.1.2 Open Submanifolds and General Foliations

While the reader can bear in mind the compact ESMs as a rolemodel on almost any occasion, we will also treat open ESMs to some degree within this thesis. So

⁽²⁾ \Subset stands for a relatively compact subset, so $A \Subset B \Leftrightarrow \text{clos}(A) \subseteq \text{int}(B)$.

we need to prepare this suitably. Further, although it is effectively sufficient to treat foliations and extensions in terms of the normal extension and foliation, it may sometimes be convenient to choose other kinds of extensions and corresponding foliations. And while we present the results in the upcoming chapters just for the normal foliation, an equivalent treatment for more general foliations and extensions is possible on most occasions as well. So we give here a short sketch of these more general choices after introducing open ESMs.

Open Subdomains of Closed Submanifolds

Obviously, any open, connected subdomain of a compact ESM is an embedded submanifold in its own right, and we can define normal space balls, tubular neighbourhood, projection, extension and foliation just by restriction. However, to make all other upcoming considerations work, we will have to state further demands for such domains in the way we are going to employ them in this thesis:

First of all, we will demand that M is an open subdomain of some $\widehat{M} \in \mathbb{M}_{\text{cp}}^k(\mathbb{R}^d)$. Furthermore, we demand that the relative boundary is made up of at most finitely many connected components $\{\Gamma_j\}_{j=1}^\ell$ such that $\Gamma_j \in \mathbb{M}_{\text{cp}}^{k-1}(\mathbb{R}^d) \cap \mathbb{M}_{\text{cp}}^{k-1}(\widehat{M})$ for all $j \in J$. We also note that each Γ_j is orientable as a submanifold of \widehat{M} . Consequently, and by the required properties of \widehat{M} , one can deduce that M has a finite inverse atlas $\mathbb{A}_M = (\psi_i, \omega_i)_{i \in I}$ such that for any $i \in I$ the following holds:

- $\omega_i \in \text{Lip}_k$ and any ψ_i is C -bounded and injective on ω_i .
- There is an inverse atlas $\mathbb{A}_{\widehat{M}} \in \mathbb{II}(\widehat{M})$ of \widehat{M} such that any pair $(\psi, \omega) \in \mathbb{A}_M$ can be obtained by restriction of a suitable pair $(\widehat{\psi}, \widehat{\omega}) \in \mathbb{A}_{\widehat{M}}$, so $\omega \subseteq \widehat{\omega}$ and $\psi = \widehat{\psi}|_\omega$.

A suitable method for the construction of such an inverse atlas can for example be deduced from [55, Sect. 3] and is given in the appendix. There, we present the construction for only one boundary connected component, but the construction generalises naturally to finitely many components.

2.17 Definition

1. A smooth embedded submanifold M of \mathbb{R}^d with dimension k that is a subdomain of some $\widehat{M} \in \mathbb{M}_{\text{cp}}^k(\mathbb{R}^d)$ as introduced above is denoted by $M \in \mathbb{M}_{\text{sd}}^k(\mathbb{R}^d)$. If a smooth embedded submanifold M of dimension k of \mathbb{R}^d is either in $\mathbb{M}_{\text{sd}}^k(\mathbb{R}^d)$ or in $\mathbb{M}_{\text{cp}}^k(\mathbb{R}^d)$, we denote this by $\mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$.
2. An inverse atlas of \widehat{M} where the stated restrictability holds will be called a *M-restrictable inverse atlas* of \widehat{M} , or just *restrictable inverse atlas*. It will be denoted by $\mathbb{A}_{\widehat{M}} \in \mathbb{II}_R(\widehat{M})$. Furthermore, we will denote the restricted inverse atlas \mathbb{A}_M of M again by $\mathbb{A}_M \in \mathbb{II}(M)$.

2.18 Remark: (1) We can presume by arguments presented in Sect. 9.1 of the appendix that we are equipped with such (restrictable) inverse atlases.

(2) Unless explicitly stated otherwise, the term ESM will also include such open domains. If they are not included, we refer to a *compact ESM* or an *ESM without boundary*, which remain as equivalent expressions within this thesis.

(3) As any relevant properties of extended inverse atlas \mathcal{U}_M for M obtained by restriction of $\mathcal{U}_{\widehat{M}} \in \mathbb{I}_N^{\text{ex}}(\widehat{M})$ are retained, we can also generalise the notation of $\mathbb{I}_N^{\text{ex}}(M)$ to these: We write $\mathcal{U}_M \in \mathbb{I}_N^{\text{ex}}(M)$ if it is obtained by restriction of $\mathcal{U}_{\widehat{M}} \in \mathbb{I}_N^{\text{ex}}(\widehat{M})$.

Notes on other Foliations and Extensions

Although we will effectively restrict ourselves in the course of this thesis to normal foliation and normal extension, this is not the only way to obtain a foliation and extension. For example and as proposed in [76], if $M = \varphi^{-1}\{0\}$ for an implicit function $\varphi : \mathbb{R}^d \rightarrow \mathbb{R}$, then the gradient $\nabla\varphi$ gives rise to gradient vector field

$$\Upsilon : U(M) \rightarrow \mathbb{R}^d, \quad \Upsilon(y) := \frac{\nabla\varphi(y)}{\|\nabla\varphi\|_2^2}$$

on $U_\varrho^\varphi(M) \subseteq U(M) \subseteq U_\varrho^\varphi(M)$, where $\varrho > \delta > 0$ is chosen such that φ is a smooth submersion on

$$U_\varrho^\varphi(M) := \{y \in \mathbb{R}^d : |\varphi(y)| \leq \varrho\}.$$

Consequently, it gives rise in turn to a uniquely and well-defined gradient flow v for the initial conditions

$$\partial_t(v(y, t)) = \Upsilon(y), \quad v(y, t) = y, y \in U_\varrho^\varphi(M)$$

by the Picard-Lindelöf theorem for any t until we reach the boundary of $U_\varrho^\varphi(M)$. Moreover, we obtain the further relation

$$\varphi(v(y, t)) = \varphi(y) + t, t \in I_y :=]-\varphi(y) - \varrho, -\varphi(y) + \varrho[.$$

The orbits $v(\xi, \cdot)$ for $\xi \in M$ then define our foliation \mathbb{F}_φ . This foliation is still orthogonal to M in the sense that any leaf for a point $\xi \in M$ is orthogonal to M at that point: the tangent (normal) space of M and the tangent (normal) space of the leaf (as a submanifold) are mutually orthogonal at ξ . Furthermore, we can directly provide a diffeomorphic map between neighbourhoods obtained by this foliation and by the normal foliation: As the normal foliation must exist also in this case, we can define for an arbitrary $y = \Psi_i(x, z) \in U(M)$ a map via

$$y = \Psi_i(x, z) \mapsto v(\psi_i(x), z)$$

which is by conception diffeomorphic and C-bounded on a sufficiently narrow $U(M)$. This relation leads to the following, more general definition:

2.19 Definition Let $\varphi : \Omega \rightarrow \mathbb{R}^d$ be a C-bounded diffeomorphism such that both $U_\varepsilon^N(M) \subseteq \Omega$ and $\varphi(x) = x$ for all $x \in M$. Let \mathbb{F}_N be the normal foliation of $U_\varepsilon^N(M)$ subordinate to M . Let $(\psi_i, \omega_i)_{i \in I} \in \mathbb{I}(M)$ be an inverse atlas of M and $(\Psi_i, \Omega_i^\varepsilon)_{i \in I} \in \mathbb{I}_N^{\text{ex}}(M)$ an inverse atlas of $U_N(M)$ for the normal foliation. Then we call the set

$$\mathbb{F} = \{\varphi(N_x^\varepsilon) : x \in M, N_x^\varepsilon = B_\varepsilon^N(x) \text{ leaf of } \mathbb{F}_N\}$$

M -foliation or just foliation of $U_\varepsilon^{\mathbb{F}}(M) = \varphi(U_\varepsilon^N(M))$. Each $F_x^\varepsilon := \varphi(N_x^\varepsilon)$ for $x \in M$ is called a leaf of \mathbb{F} . We call this foliation an *orthogonal foliation* if for any $x \in M$ the tangent space $T_x M$ and the tangent space $T_x F_x^\varepsilon$ of the leaf F_x^ε of \mathbb{F} containing x are mutually orthogonal. We call the foliation a *linear foliation* if any leaf is subset of a κ -dimensional affine subspace of \mathbb{R}^d and φ is a linear map on any leaf of the normal foliation.

2.20 Example: A particularly interesting foliation that is not orthogonal but linear can be obtained for all $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ that allow for a well-defined projection onto the sphere in \mathbb{R}^d , for example a compact hypersurface M that contains a star-shaped domain: The vector field obtained by normalising the position of any point gives a suitable vector field that is never tangent and as smooth as M . By compactness it is then not hard to see that there is $\varepsilon > 0$ such that for any $y \in M$ and $v(y) := y/\|y\|_2$ it holds $\langle v(y), \tau(y) \rangle \geq \varepsilon$ for any $\tau(y) \in T_y M$. In case of a hypersurface, this direction can be used directly to obtain a foliation, where one just replaces the normal direction $v(\psi(x))$ in the extended parameterisation for the normal foliation by the direction $v(\psi(x))$. Then we could parameterise even all of $\mathbb{R}^d \setminus \{0\}$ in the form

$$\Psi_i^v(x, z) := \psi_i(x) + z v(\psi_i(x)), \quad z \in]-\|\psi(x)\|_2, \infty[.$$

In case of higher codimension, we would just have to choose further (fixed) directions that are never tangent and linearly independent of the "point direction" $v(\psi_i(x))$. This is easy however, as by the required uniqueness of projection of the ESM onto the sphere there are multiple valid choices. The resulting foliation can be made linear by suitable parameterisation. Moreover, it can yield considerably larger neighbourhoods if necessary, as in fact the whole line from zero through the point on the ESM can serve as a leaf.

We can in fact use any foliation to define a projection $\Pi_M^{\mathbb{F}} : U^{\mathbb{F}}(M) \rightarrow M$ via

$$\Pi_M^{\mathbb{F}} : z = \Psi_i^{\mathbb{F}}(x, z) \mapsto x,$$

where we define $\Psi_i^{\mathbb{F}}(x, z) = \varphi_{\mathbb{F}}(\Psi_i(x, z))$ for Ψ_i according to standard extended inverse atlas $(\Psi_i, \Omega_i^{\varepsilon})_{i \in I} \in \Pi_N^{\text{ex}}(M)$ based on the normal foliation and extension. Thereby, we can also define an extension $E_{\mathbb{F}} : f \mapsto f \circ \Pi_M^{\mathbb{F}}$.

2.21 Remark: (1) Although the preferred extension in our theory is the normal extension, it is sometimes in practice more convenient to use a different extension. If for example the maximal extent of a tubular neighbourhood of M with the closest point property is small, then a different extension based on for example the gradient field construction above can lead to a significantly larger $U^{\mathbb{F}}(M)$.

(2) Again, the directional derivative of an extension $E_{\mathbb{F}}f = f \circ \Pi_M^{\mathbb{F}}$ vanishes along the leaves of \mathbb{F} .

2.22 Definition A regularity preserving extension $F : U(M) \rightarrow \mathbb{R}$ of a function $f \in C^1(M, \mathbb{R})$ is called an *orthogonal extension* if $\frac{\partial F}{\partial v}(x) = 0$ for any $v \in N_x M$ and any $x \in M$.

2.23 Remark: We do not demand that this directional derivative vanishes in points *within the whole normal space* for an orthogonal extension — that property is effectively reserved for the normal foliation.

2.2 Function Spaces on Embedded Submanifolds

We now make a brief tour over function spaces. The most common spaces in approximation theory are usually either spaces of continuous differentiability of certain order — the classical spaces in which approximation theory used to take place — or their closures under certain integral norms, so *Sobolev spaces*. And as soon as one is taking the restriction RF of such a function F to subspaces and submanifolds (called a *trace* $T_M F$ of F), one naturally comes across *fractional Sobolev spaces*. Since nowadays practical approximation theory usually takes place in Sobolev spaces, we shall concentrate on these, and also give a short treatment of fractional order spaces as well.

We start by giving a definition based on completion — among numerous other ways to define these space — where we follow [1, 2]:

2.24 Definition 1. Let $\Omega \in \text{Lip}_d^*$, $m \in \mathbb{N}_0$, $p \in [1, \infty[$ and ∂^{α} be the partial derivative w.r.t. multi-index α . Then we define the norm

$$\|f\|_{W_p^m(\Omega)} := \left(\int_{\Omega} \sum_{\mu=0}^m \sum_{|\alpha|=\mu} |\partial^{\alpha} f|^p \right)^{1/p}$$

on the space $C^\infty(\Omega)$ of all smooth functions. We define the Sobolev space $W_p^m(\Omega)$ as the completion of the subspace of $C^\infty(\Omega)$ where this norm is finite.

2. Let $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ be equipped with a finite inverse atlas $\mathbb{A}_M = \{(\psi_i, \omega_i)\}_{i=1}^n \in \mathbb{II}(M)$. Then we define the Sobolev space $W_p^m(M)$ as the completion of the set of all smooth functions $f : M \rightarrow \mathbb{R}$ where

$$\|f\|_{W_p^m(M)} := \sum_{i=1}^n \|f \circ \psi_i\|_{W_p^m(\omega_i)} < \infty.$$

3. In all cases, we will usually write H^m for W_2^m . Furthermore, L_p denotes the case $m = 0$, as any of these is in particular a *Lebesgue space*.

2.25 Remark: Different choices of the inverse atlas yield different, yet equivalent norms on a distinct ESM. In particular, if an ESM $M \in \mathbb{M}_{\text{sd}}^k(\mathbb{R}^d)$ is an open domain in another ESM $\widehat{M} \in \mathbb{M}_{\text{cp}}^k(\mathbb{R}^d)$, then the definition of the Sobolev spaces for M is not directly obtained as a restriction of the definition for \widehat{M} , in contrast to the Euclidean case. But by changing to the restrictable inverse atlas, we can achieve this. In the following, we will always presume the inverse atlas to be fixed if not explicitly stated otherwise, and restrictable if open ESMs are considered.

For the relations and embeddings between these spaces, also on ESMs, we refer the reader to the appendix and state here just that the usual Sobolev and Rellich-Kondrachov embeddings hold. We proceed instead with some results that yield an equivalent norm for integer order Sobolev spaces on ESMs based on normal extensions as introduced above. The statement and proof are very similar to the results given in [76] or [82], and we postpone the proof to the appendix:

2.26 Theorem *If $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ is contained in a family $U_h(M)$ of tubular neighbourhoods with $0 < h < h_0$, then there are fixed $a_1, a_2 > 0$ independent of h such that for any $F \in W_p^m(U_h(M))$ and inverse atlas $\mathbb{U}_M = (\Psi_i, \Omega_i^h)_{i \in I} \in \mathbb{II}_N^{\text{ex}}(M)$ of $U_h(M)$*

$$a_1 \|F\|_{W_p^m(U_h(M))} \leq \sum_{i \in I} \|F \circ \Psi_i\|_{W_p^m(\Omega_i^h)} \leq a_2 \|F\|_{W_p^m(U_h(M))}.$$

Additionally, it holds for any $f \in W_p^m(M)$ and suitable b_1, b_2 independent of h

$$b_1 h^{k/p} \|f\|_{W_p^m(M)} \leq \|E_N f\|_{W_p^m(U_h(M))} \leq b_2 h^{k/p} \|f\|_{W_p^m(M)}.$$

In particular, a specialised version of this theorem emphasises the relation between different extents of the tubular neighbourhoods that are still proportional to some parameter $0 < h < h_0$:

2.27 Corollary *In the setting of the last result, let $a, b > 0$. Then it holds for all $0 < h < h_0$, any $f \in W_p^m(M)$ and suitable $c_1, c_2 > 0$ independent of h, a, b that*

$$c_1 a^{-\kappa/p} h^{-\kappa/p} \|E_N f\|_{W_p^m(U_{ah}(M))} \leq \|f\|_{W_p^m(M)} \leq c_2 b^{-\kappa/p} h^{-\kappa/p} \|E_N f\|_{W_p^m(U_{bh}(M))}.$$

Consequently, all three norms are equivalent for fixed choices of a and b .

As soon as it comes to ESMs, one is naturally confronted with the problem of taking traces of functions defined in the ambient space. In order to keep as much regularity as possible, this will necessarily lead to leaving the Sobolev spaces of integer order behind, and we will have to turn to more elaborate constructions. This leads to certain fractional order spaces and in the end also to Besov spaces. One way to define suitable fractional order spaces — with the alternative naming *Slobodeckij spaces* — is as follows (cf. [1, 2, 32, 98, 96, 100]), where we restrict ourselves to the Hilbert case as the only one we are effectively interested in:

2.28 Definition Let $\Omega \in \text{Lip}_d^*$. Then we define for $0 < s < 1, m \in \mathbb{N}_0$ the norm

$$\|f\|_{H^{m+s}} := \|f\|_{H^m} + \left(\int_{\Omega \times \Omega} \sum_{|\alpha|=m} \frac{|\partial^\alpha f(x) - \partial^\alpha f(z)|^2}{\|x - z\|_2^{d+2s}} dx dz \right)^{1/2}$$

on the space of all smooth functions where this norm is finite. We define the fractional Sobolev space (or *Slobodeckij space*) $H^{m+s}(\Omega)$ as their completion in that norm. We further define $H^{m+s}(M)$ for $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ as above by completion under

$$\|f\|_{H^{m+s}(M)} := \sum_{i=1}^n \|f \circ \psi_i\|_{H^{m+s}(\omega_i)}.$$

for a finite inverse atlas $\mathbb{A}_M = \{(\psi_i, \omega_i)\}_{i=1}^n \in \mathbb{I}(M)$.

The following fact about Sobolev and Slobodeckij spaces due to [32],[87], [93, §3, Thm. 5], [99] is of significant importance. Thereby, we can directly transfer a property that holds in \mathbb{R}^d for one of those spaces also into the respective space on a subdomain $\Omega \in \text{Lip}_d$:

2.29 Proposition If $\Omega \in \text{Lip}_d$ and $1 \leq p < \infty$, then there is an extension operator $E_\Omega : W_p^m(\Omega) \rightarrow W_p^m(\mathbb{R}^d)$ independent of $0 \leq m < \infty$ such that for any $f \in W_p^m(\Omega)$ and fixed $c > 0$

$$\|E_\Omega f\|_{W_p^m(\mathbb{R}^d)} \leq c \|f\|_{W_p^m(\Omega)}.$$

The same holds also for $H^r(\Omega)$, and the operator is independent of $0 \leq r < \infty$.

As stated in the introduction, we present a more thorough treatment of these spaces on submanifolds in the appendix. Here, we restrict ourselves to the statement that the usual properties like Sobolev embeddings or norm equivalence under diffeomorphic maps hold. Proofs or references are given in the appendix. There, we also present some further consequences of function space interpolation in our setting, a short note on Besov spaces and the proofs for the statements in the re-

maining sections of this chapter. At this point, we shall only give one very important property that is deduced in the appendix as well, the *interpolation property*:

2.30 Proposition *Let $\Omega_1 \in \text{Lip}_{d_1}^*$, $\Omega_2 \in \text{Lip}_{d_2}^*$. Let $r = \theta r_1 + (1-\theta)r_2$ for $\theta \in]0, 1[$ and reals $0 \leq r_1 \leq r_2 < \infty$ and let $\varrho = \theta \varrho_1 + (1-\theta)\varrho_2$ for reals $0 \leq \varrho_1 \leq \varrho_2 < \infty$. If $\Lambda : H^{r_i}(\Omega_1) \mapsto H^{\varrho_i}(\Omega_2)$ is bounded for $i = 1, 2$, then $\Lambda : H^r(\Omega_1) \mapsto H^\varrho(\Omega_2)$ is bounded as well and*

$$\|\Lambda\|_{H^r \rightarrow H^\varrho} \leq c_\Omega \|\Lambda\|_{H^{r_1} \rightarrow H^{\varrho_1}}^\theta \|\Lambda\|_{H^{r_2} \rightarrow H^{\varrho_2}}^{(1-\theta)}.$$

If a family $\{\Lambda_h\}_{0 < h < h_0}$ of such operators satisfies

$$\|\Lambda_h\|_{H^{r_1} \rightarrow H^{\varrho_1}}^\theta \leq c_1 h^{\lambda_1} \quad \text{and} \quad \|\Lambda_h\|_{H^{r_2} \rightarrow H^{\varrho_2}}^{(1-\theta)} \leq c_2 h^{\lambda_2},$$

then we have in particular the relation $\|\Lambda_h\|_{H^r \rightarrow H^\varrho} \leq c h^{\lambda_1 \cdot \theta + \lambda_2 \cdot (1-\theta)}$.

2.2.1 Trace Theorems

The spaces just introduced give us the key to take traces of functions $F : U(M) \rightarrow \mathbb{R}$ on ESMs. These results are usually given for $\Omega \in \text{Lip}_d$ or \mathbb{R}^d and $\Omega^k = \Omega \cap (\mathbb{R}^k \times \{0\}^{d-k})$ or $\mathbb{R}^k \times \{0\}^{d-k}$, but since we have a finite set of Lipschitz parameter spaces and C-bounded parameterisations, they generalise directly to ESMs.

To this end, we define now the restriction $T_M : C^\infty(\mathbb{R}^d) \rightarrow C^\infty(M)$ pointwise and for the fractional and integer Sobolev spaces via completion. Then we obtain the following trace theorems, for which we present literature references and proofs of certain generalising aspects in Sect. 9.2.5 of the appendix.

2.31 Theorem — Integer Trace Theorem —

1. *Let $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ be equipped with finite inverse atlas $\mathbb{A}_M = \{(\psi_i, \omega_i)\}_{i \in I} \in \mathbb{II}(M)$ and let $U(M) \in \text{Lip}_d$ be some ambient tubular neighbourhood of M with fixed extent $\varrho > 0$. Let $F \in W_p^m(U(M))$ for some $1 \leq p < \infty$ and $m \in \mathbb{N}$. Then $T_M F \in W_p^\mu(M)$ for any $\mu \in \mathbb{N}_0$ with $\mu < m - \frac{d-k}{p}$ ($\mu \leq m - \frac{d-k}{p}$ in case $p = 1$) and*

$$\|T_M F\|_{W_p^\mu(M)} \leq c \|F\|_{W_p^m(U(M))}.$$

2. *Let $f \in W_p^m(M)$ for some $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ and some $1 \leq p < \infty$ and $m \in \mathbb{N}$. Take some open and bounded $M_0 \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ with $M_0 \Subset M$ that has nonempty smooth boundary Γ . Then $T_\Gamma f \in W_p^\mu(\Gamma)$ for any $\mu < m$ and*

$$\|T_\Gamma f\|_{W_p^\mu(\Gamma)} \leq c \|f\|_{W_p^m(M_0)}.$$

Things become more involved when one is willing to consider fractional orders. The gain we can hope for in that setting is that if we consider fractional spaces, the loss of regularity might be considerably lower than implied by the integer case, and so we could hope for tighter relations in future approximation results.

Unfortunately, taking traces of Sobolev spaces will not necessarily bring you into a Sobolev space as the most regular space to end up in, not even a fractional one. But there is one important exception to this: Whenever $p = 2$, then everything coincides and we are in a Slobodeckij space. So this is the case we go for:

2.32 Theorem — Fractional Trace Theorem —

Let $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ have finite inverse atlas $\mathbb{A}_M = \{(\psi_i, \omega_i)\}_{i \in I} \in \mathbb{I}(M)$ and let $U(M) \in \mathbb{Lip}_d$ be some tubular neighbourhood of M with fixed extent $\varrho > 0$ and extended inverse atlas $\{(\Psi_i, \Omega_i)\}_{i \in I} \in \mathbb{I}_N^{\text{ex}}(M)$ subordinate to \mathbb{A}_M . Let $F \in H^r(U(M))$ for $r > \frac{d-k}{2}$. Then $T_M F \in H^\varrho(M)$ for $\varrho = r - \frac{d-k}{2} > 0$ and

$$\|T_M F\|_{H^\varrho(M)} \leq c \|F\|_{H^r(U(M))}.$$

Conversely, there is also a bounded extension operator $E_M^U : H^\varrho(M) \rightarrow H^r(U(M))$, so for any $g \in H^\varrho(M)$

$$\|E_M^U g\|_{H^r(U(M))} \leq c \|g\|_{H^\varrho(M)}.$$

Again, this extension operator is independent of ϱ and thus universally applicable for any $\varrho > 0$ and $r = \varrho + \kappa/2$. All statements remain valid if one replaces $U(M)$ by M and M by some ESM $\Gamma \in \mathbb{M}_{\text{bd}}^\ell(M)$ for $0 < \ell < k$.

The proof of this theorem for ESMs, given in the appendix by deduction from results on linear subspaces, yields in particular the following additional result:

2.33 Corollary — Chart Trace Theorem —

In the setting of the last theorem it holds for any pair (ψ, ω) from the inverse atlas $\mathbb{A}_M \in \mathbb{I}(M)$, corresponding $(\Psi, \Omega) \in \mathbb{U}_M \in \mathbb{I}_N^{\text{ex}}(M)$ and $F \in H^r(U(M))$ that

$$\|T_\omega(F \circ \Psi)\|_{H^\varrho(\omega)} \leq c \|F\|_{H^r(\Psi(\Omega))} \leq c \|F\|_{H^r(U(M))}.$$

Conversely, there is a bounded extension operator $E_\omega^U : H^\varrho(\omega) \rightarrow H^r(U(M))$ such that for any g such that $g \circ \psi \in H^\varrho(\omega)$

$$\|E_\omega^U g\|_{H^r(U(M))} \leq c \|(g \circ \psi)\|_{H^\varrho(\omega)}.$$

2.34 Remark: (1) All results on traces also hold for any other Lipschitz neighbourhood of an ESM that contains a tubular neighbourhood of fixed extent, and

the extension results for any Lipschitz neighbourhood of an ESM that is itself contained in such a tubular neighbourhood. Both come directly by restriction.

(2) Note that we cannot say anything about traces when $\varrho = 0$. There, the respective results will in fact fail; and while there are other conditions under which one can indeed achieve a trace (cf. [88, Cor. 3.17 etc.]), these conditions will no longer fit into our theory as they apply to $p \leq 1$ only, so we omit them here.

Nonetheless, there is at least one specific situation where we have some kind of result when taking traces even in case $\varrho = 0$: Namely if we start from M in the right manner. Then we can give a result on traces that is concerned with extensions based on foliations. Its main purpose is to point out that the trace of a function extended from an ESM into a suitable neighbourhood by the normal (or any other foliation-based) extension is the function we started with:

2.35 Theorem — Foliation Trace Theorem —

Let $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ have the finite inverse atlas $\mathbb{A}_M = \{(\psi_i, \omega_i)\}_{i=1}^n \in \mathbb{II}(M)$ and let $U(M) \in \text{Lip}_d$ be some tubular neighbourhood of M with fixed extent $\varrho > 0$. If then $f \in W_p^m(M)$ it holds $T_M E_N f \in W_p^m(M)$ and

$$\|f - T_M E_N f\|_{W_p^m(M)} = 0.$$

We also have the following result, which gives us an universal extension operator for ESMs that corresponds to the extensions from Euclidean domains to \mathbb{R}^d :

2.36 Theorem — Manifold Extension Theorem —

Let $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ be equipped with inverse atlas $\mathbb{A}_M = \{(\psi_i, \omega_i)\}_{i=1}^n \in \mathbb{II}(M)$. Let further $M_0 \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ be an open subdomain $M_0 \Subset M$ that is an ESM of dimension k in its own right. Then there is an extension operator $E : H^r(M_0) \rightarrow H^r(M)$ such that for any $r > 0$ and any $g \in H^r(M_0)$

$$\|Eg\|_{H^r(M)} \leq c \|g\|_{H^r(M_0)}.$$

This holds also if one replaces M_0 by an arbitrary parameter space ω with corresponding parameterisation ψ according to the inverse atlas in the sense

$$\|E_\omega^M g\|_{H^r(M)} \leq c \|g \circ \psi\|_{H^r(\omega)}.$$

2.2.2 Friedrichs' Inequality

Friedrichs' Inequality is an important tool in functional analysis and particularly in the treatment of partial differential equations. For us, it will be important in bounding $F - E_N T_M F$ for suitable functions F defined on some $U(M)$. However, a clear drawback in particular in this application is the restriction in the dimension of the ambient space, as the offset to the ESM dimension must not be greater than one in the classical formulation of the inequality. Since we are going to investigate ESMs also in cases where the codimension is greater than one, there is a natural need for an extended result. We present it here, while we postpone the technical proof to Sect. 9.2.6 in the appendix:

2.37 Theorem — Multicodimensional Friedrichs' Inequality —

Let $\omega \in \text{Lip}_k$ and let $\Omega_h = \omega \times B_h^k[0]$ for $0 < h < h_0$. Let $F \in W_p^k(\Omega_h)$ for some $1 \leq p < \infty$ be a continuous function that vanishes on ω . Then we have the relation

$$\|F\|_{L_p(\Omega_h)}^p \leq c \sum_{\ell=1}^k h^{p \cdot \ell} \sum_{\substack{|\alpha|=\ell \\ \alpha_1=\dots=\alpha_k=0}} \|\partial^\alpha F\|_{L_p(\Omega_h)}^p.$$

We also give a tightened variant of this relation for functions that are polynomials of fixed degree on each $\{x\} \times B_h^k[0]$, where the codimension plays no role anymore. Again, the proof is postponed to the appendix.

2.38 Theorem — Leafwise Polynomial Friedrichs' Inequality —

Let $\omega \in \text{Lip}_k$ and let $\Omega_h = \omega \times B_h^k[0]$. Let $F \in W_p^1(\Omega_h)$ for some $1 \leq p < \infty$ be a continuous function that vanishes on ω . Let further the restriction of F to any $\{x\} \times B_h^k[0]$ be a polynomial of maximal degree $n \in \mathbb{N}$. Then we have the relation

$$\|F\|_{L_p(\Omega_h)}^p \leq c h^p \sum_{\substack{|\alpha| \geq 1 \\ \alpha_1=\dots=\alpha_k=0}} \|\partial^\alpha F\|_{L_p(\Omega_h)}^p$$

for a constant $c = c(n) > 0$ independent of F and h .

2.39 Remark: While Theorem 2.37 would work out in the same manner also for other foliations, the latter result Theorem 2.38 requires the foliation to be linear, as in this case the restriction of a polynomial to a leaf is always a polynomial of the same order in both image and preimage of the foliation parameterisation.

Chapter 3

Ambient Approximation Theory

The core of this chapter is the investigation of approximation operators A^M for functions on ESMs that are defined by a roundtrip over some ambient neighbourhood $U(M)$. Essentially, they all apply the following common concept: Given an approximation operator A on some function space defined in $U(M)$, we make the choice

$$A^N = T_M A E_N$$

or more generally $A^F = T_M A E_F$ for some other foliation-based extension E_F . By this approach, we will be able to transfer many of the extrinsic properties of A to the intrinsic setting. In particular, if we have a family $(A_h)_{0 < h < h_0}$ with approximation order h^λ , we ask what we can say about the approximation order of the corresponding $(A_h^N)_{0 < h < h_0}$. We will see that under mild additional assumptions and for suitable approximation spaces like tensor product splines (TP-splines), we will be able to maintain the approximation order also in the intrinsic setting.

To be more precise, we will first present results that can be stated for general classes of approximation operators, before we turn to the important concepts of quasi-interpolation and quasi-projection. These will be discussed in further detail and exemplified by suitable operators for TP-splines, and we will finish this chapter by providing results for approximation of the derivatives along the *normals* of M , which will turn out to be crucial in upcoming chapters.

In the whole course of this chapter, M is an ESM of dimension k and codimension κ , and $U(M)$ is an ambient tubular neighbourhood equipped with the closest point property (or its equivalent for another foliation based projection). Both are equipped with their respective finite C -bounded Lipschitz inverse atlases. All the results presented for E_N remain valid if one replaces our standard example E_N with some other foliation based extension E_F if not explicitly stated otherwise.

3.1 General Approximation Operators

We do already have two tools at hand that can provide us with approximation results for restrictions: One is the trace theorem, the other is our version of Friedrichs' inequality.

However, if we look for an application of the trace theorem, then we loose some regularity and would therefore also expect to loose some approximation order: If we have $A_h^N = T_M A_h E_N$ and

$$\|E_N f - A_h E_N f\|_{H^e(U(M))} \leq c h^{r-e} \|E_N f\|_{H^r(U(M))},$$

we could only deduce the presumably suboptimal relation

$$\|f - A_h^N f\|_{H^{e-\frac{k}{2}}(M)} \leq c h^{r-e} \|f\|_{H^r(M)}.$$

We could overcome this by application of the universal extension $E_M : H^r(M) \rightarrow H^{r+\frac{d-k}{2}}(U(M))$ and deduce from

$$\|E_M f - A_h E_M f\|_{H^{e+\frac{k}{2}}(U(M))} \leq c h^{r-e} \|E_M f\|_{H^{r+\frac{k}{2}}(U(M))}$$

that for $A_h^M := T_M A_h E_M$

$$\|f - A_h^M f\|_{H^e(M)} \leq c h^{r-e} \|f\|_{H^r(M)},$$

but this extension is hardly ever known in practice. And that approach has another drawback: In contrast to the use of E_N , the use of E_M does usually not imply approximately vanishing normal derivatives, which will turn out to be crucial in forthcoming chapters. So these direct results are rather unpleasant: We have either to expect some loss in the approximation order or we have to rely on an extension operator that is hardly ever known explicitly. Therefore, we need to take another approach. This will indeed be capable of maintaining approximation orders while employing extensions that are practically applicable, and it relies on the following definition:

3.1 Definition Let $(U_{ah}(M))_{h < h_0}$, $(U_{bh}(M))_{h < h_0}$ be two families of tubular neighbourhoods for fixed $0 < a \leq b < \infty$. Let $F(U_{bh}(M))$, $G(U_{ah}(M))$ be function spaces. Let F be an arbitrary function that is contained in $F(U_{bh}(M))$ and $G(U_{ah}(M))$ for all $h < h_0$. Then a family $(A_h)_{h < h_0}$ of approximation operators mapping $F(U_{bh}(M))$ to $G(U_{ah}(M))$ for each $h < h_0$ is called *local relative to M* with approximation order λ if it satisfies the relation

$$\|F - A_h F\|_{G(U_{ah}(M))} \leq c h^\lambda \|F\|_{F(U_{bh}(M))}$$

with a generic constant $c > 0$ that is independent of F and h in particular.

3.2 Remark: We will see later that for appropriate choices of the neighbourhoods, suitable quasi-interpolation approaches for TP-splines are local relative to \mathbf{M} for ESMs without boundary.

The next theorem, which is a generalisation of results from [75, 76, 82] to a setting with higher codimensions, is now giving us the desired reproduction of approximation orders. But that comes at the price of increasingly limited range as the codimension increases:

3.3 Theorem *Let $(U_{ah}(\mathbf{M}))_{h < h_0}, (U_{bh}(\mathbf{M}))_{h < h_0}$ be two families of tubular neighbourhoods with $0 < a \leq b < \infty$ and let $m \in \mathbb{N}$, $1 \leq p < \infty$. Let $(A_h)_{h < h_0}$ be a family of approximation operators local relative to \mathbf{M} that map $W_p^m(U_{bh}(\mathbf{M}))$ into $W_p^\mu(U_{ah}(\mathbf{M}))$ for fixed integer $\mu \in \{0, \dots, m - \kappa\}$. Let further for any $\lambda \in \{\mu, \dots, \mu + \kappa\}$ hold*

$$\|F - A_h F\|_{W_p^\lambda(U_{ah}(\mathbf{M}))} \leq c h^{m-\lambda} \|F\|_{W_p^m(U_{bh}(\mathbf{M}))}.$$

Then $A_h^N := T_M A_h E_N$ satisfies for any $f \in W_p^m(\mathbf{M})$ the relation

$$\|f - A_h^N f\|_{W_p^\mu(\mathbf{M})} \leq c h^{m-\mu} \|f\|_{W_p^m(\mathbf{M})}.$$

Proof: We give the proof using ideas of [75, 76, 82] for the case of codimension one. To simplify notation in the subsequent arguments, we make the abbreviations $\vec{F} = E_N f$, $F_h = A_h \vec{F}$, $\vec{F}_h = E_N T_M F_h$, $U_h = U_h(\mathbf{M})$, $U_{ah} = U_{ah}(\mathbf{M})$, $U_{bh} = U_{bh}(\mathbf{M})$. Then we choose an arbitrary single pair (ψ, ω) from inverse atlas $\mathbb{A}_M \in \Pi(\mathbf{M})$ and corresponding pairs (Ψ, Ω_{ah}) , (Ψ, Ω_{bh}) for the parameterisations of the neighbourhoods by the normal foliation. By the norm equivalences of Theorem 2.26 and the fact that $a > 0$ is fixed, we obtain the relation

$$\begin{aligned} \|f - A_h^N f\|_{W_p^\mu(\psi(\omega))} &\leq c h^{-\kappa/p} \|\vec{F} - \vec{F}_h\|_{W_p^\mu(\Psi(\Omega_{ah}))} \\ &\leq c h^{-\kappa/p} \left(\|\vec{F} - F_h\|_{W_p^\mu(\Psi(\Omega_{ah}))} + \|F_h - \vec{F}_h\|_{W_p^\mu(\Psi(\Omega_{ah}))} \right). \end{aligned} \quad (3.3.1)$$

The first summand there can be bounded by our hypothesis as

$$\begin{aligned} \|\vec{F} - F_h\|_{W_p^\mu(\Psi(\Omega_{ah}))} &\leq \|\vec{F} - F_h\|_{W_p^\mu(U_{ah})} \leq c h^{m-\mu} \|\vec{F}\|_{W_p^m(U_{bh})} \\ &\leq c h^{\kappa/p} h^{m-\mu} \|f\|_{W_p^m(\mathbf{M})} \leq c h^{m-\mu+\kappa/p} \|f\|_{W_p^m(\mathbf{M})}. \end{aligned} \quad (3.3.2)$$

For the second summand we have to work a bit harder: We obtain once again by equivalence of Sobolev norms under diffeomorphisms that

$$\begin{aligned}\|F_h - \vec{F}_h\|_{W_p^\mu(\Psi(\Omega_{ah}))} &= \sum_{|\beta| \leq \mu} \|\partial^\beta(F_h - \vec{F}_h)\|_{W_p^\mu(\Psi(\Omega_{ah}))} \\ &\leq c \sum_{|\alpha| \leq \mu} \|\partial^\alpha(F_h \circ \Psi - \vec{F}_h \circ \Psi)\|_{W_p^\mu(\Omega_{ah})}.\end{aligned}\quad (3.3.3)$$

Now we partition the multi-index $\alpha = (\alpha_1, \dots, \alpha_d)$ into $\alpha = (\alpha_{\underline{k}}, \alpha_{\bar{k}})$, where $\alpha_{\underline{k}}$ are the first k entries, and $\alpha_{\bar{k}}$ are the last κ entries. Then we distinguish two cases: Case one is that $|\alpha_{\bar{k}}| > 0$. In that case, we first clarify that for $f_h := T_M F_h$, the very definition of E_N yields $(E_N f_h)(\Psi(x, z)) = f_h(\psi(x))$. Hence we have

$$\partial_x^{\alpha_{\bar{k}}} \partial_z^{\alpha_{\bar{k}}} (\vec{F}_h \circ \Psi) = 0.$$

Using the same argument again we obtain $\partial_x^{\alpha_{\bar{k}}} \partial_z^{\alpha_{\bar{k}}} (\vec{F} \circ \Psi) = 0$, so in particular

$$\partial_x^{\alpha_{\bar{k}}} \partial_z^{\alpha_{\bar{k}}} (F_h \circ \Psi - \vec{F}_h \circ \Psi) = \partial_x^{\alpha_{\bar{k}}} \partial_z^{\alpha_{\bar{k}}} (F_h \circ \Psi - \vec{F} \circ \Psi).$$

Now we can exploit the approximation power of A_h : Because of norm equivalence under diffeomorphisms, the norm equivalences of Theorem 2.26 and because $|\alpha| \leq \mu$ we have

$$\begin{aligned}\|\partial^\alpha(F_h \circ \Psi - \vec{F} \circ \Psi)\|_{L_p(\Omega_{ah})} &\leq c \|F_h - \vec{F}\|_{W_p^\mu(\Psi(\Omega_{ah}))} \leq c \|F_h - \vec{F}\|_{W_p^\mu(U_{ah}(M))} \\ &\leq c h^{m-\mu} \|\vec{F}\|_{W_p^m(U_{bh}(M))} \leq c h^{m-\mu+\kappa/p} \|f\|_{W_p^m(M)}.\end{aligned}\quad (3.3.4)$$

In the second case we have $|\alpha_{\bar{k}}| = 0$. We abbreviate $R_h := F_h \circ \Psi - \vec{F}_h \circ \Psi$ and find all the requirements of the multicodimensional Friedrichs' inequality from Theorem 2.37 fulfilled. So we obtain

$$\|\partial_x^{\alpha_{\bar{k}}} R_h\|_{L_p(\Omega_{ah})}^p \leq c \sum_{\ell=1}^K h^{p \cdot \ell} \sum_{|\beta|=\ell} \|\partial_x^{\alpha_{\bar{k}}} \partial_z^\beta R_h\|_{L_p(\Omega_{ah})}^p.$$

Proceeding as before in (3.3.4) for any β , since we still have $|\alpha| + |\beta| \leq |\alpha| + \kappa \leq \mu + \kappa$ but now with some derivative in the last κ coordinates, we obtain as in (3.3.4) that

$$\|\partial_x^{\alpha_{\bar{k}}} \partial_z^\beta R_h\|_{L_p(\Omega_{ah})}^p \leq \|\partial_x^{\alpha_{\bar{k}}} \partial_z^\beta (F_h \circ \Psi - \vec{F} \circ \Psi)\|_{L_p(\Omega_{ah})}^p \leq c h^{(m-\mu-|\beta|)p+\kappa} \|f\|_{W_p^m(M)}^p,$$

and so by summation

$$\|\partial_x^{\alpha_{\bar{k}}} R_h\|_{L_p(\Omega_{ah})}^p \leq c \sum_{\ell=1}^K h^{p \cdot \ell} \sum_{|\beta|=\ell} h^{(m-\mu-\ell)p+\kappa} \|f\|_{W_p^m(M)}^p \leq c h^{(m-\mu)p+\kappa} \|f\|_{W_p^m(M)}^p.$$

Again by the norm equivalence of Theorem 2.26 and regardless of the particular choice of α , we obtain the relation

$$\|\partial^\alpha(F_h \circ \Psi - \vec{F}_h \circ \Psi)\|_{L_p(\Omega_{ah})} \leq h^{m-\mu+\kappa/p} \|f\|_{W_p^m(M)}.$$

Reinserting into (3.3.1) and taking all necessary sums over all inverse atlas elements yields the desired result, as the inverse atlas was finite by assumption. \square

3.4 Remark: The restriction in terms of κ is the main drawback of this result, as it can restrict the applicable norms significantly. Later in this chapter, we will be able to give an improved result for TP-splines and linear foliations that reduces this loss to 1, regardless of the actual codimension κ .

3.2 Quasi-Projection and Polynomial Reproduction

3.2.1 Definition and Approximation Power

The concept of *quasi-interpolation* (and more specifically *quasi-projection*, cf. e.g. [68, 89]) is vital to many approximation results in univariate and multivariate settings, and it is inevitably encountered alongside the concept of *polynomial reproduction*. The basic idea for both is simple, and the theoretical results achievable thereby have important practical consequences in many approximation methods, one of which, based on tensor product splines, we have already announced to revise in further detail hereafter. But before we come to that, we will briefly revise the general concepts of quasi-interpolation and quasi-projection. We begin with the following definition (cf. [68]):

3.5 Definition Let F be an arbitrary Banach space of functions. Let $(\varphi_i)_{i \in I}$ be a family of linearly independent elements of F that span a subspace F_1 and satisfy $\|\varphi_i\|_F \leq b$ for fixed b and any $i \in I$. Let further $(\Lambda_i)_{i \in I}$ be a family of uniformly bounded functionals on F , so $\|\Lambda_i\| < c$ for some global constant $c > 0$. Then the corresponding quasi-interpolant for any $f \in F$ is given as

$$Qf = \sum_{i \in I} \Lambda_i(f) \cdot \varphi_i.$$

If we take the special case of Lebesgue spaces with index $p \in]1, \infty[$ over \mathbb{R}^d and choose its Hölder dual $p^* = p/(p-1)$, then a *quasi-projection* is the operation

$$Qf = \sum_{i \in I} \langle f, \varphi_i^* \rangle \cdot \varphi_i \text{ with } \langle f, \varphi_i^* \rangle = \int f \cdot \varphi_i^*,$$

for functions $\{\varphi_i^*\}_{i \in I} \subseteq L_{p^*}(\mathbb{R}^d)$ with $\|\varphi_i^*\|_{L_{p^*}} \leq b$. The quasi-projection is further called a *local quasi-projection* if there is a fixed $a_0 > 0$ and a set of points $\{\zeta_i\}_{i \in I}$ such that any cube of unit length in \mathbb{R}^d contains at most n_0 of these points for a fixed $n_0 \in \mathbb{N}$ and it holds

$$\text{supp } \varphi_i \cup \text{supp } \varphi_i^* \subseteq [-a_0, a_0]^d + \zeta_i.$$

3.6 Remark: Fixed quasi-interpolation operators Q can yield others by simple scaling, and provided the operators are scaled suitably, the operator norms of Λ_i and its h -scaled version $\Lambda_{i,h}$ coincide. In particular (cf. [68]), fixed quasi-projection operators Q yield arbitrary ones by scaling and we obtain for $1/p + 1/p^* = 1$

$$Q_h f = \sum_{i \in I} \langle f, h^{-d/p^*} \varphi_i^*(\cdot/h) \rangle \cdot h^{-d/p} \varphi_i(\cdot/h).$$

The respective spaces spanned by the $\{\varphi_i(\cdot/h)\}$ will consequently be denoted by

$$F_h := \{\varphi_i(\cdot/h) : i \in I\}.$$

Common examples of function spaces and quasi-interpolation techniques feature particularly splines (cf. [81, 89] and see below) and also for example *moving least squares* (cf. [105, Ch. 4]). Both examples also come along with the second concept featured in the section title, the reproduction of polynomials. In fact it is this property that makes up the key ingredient of their approximation power:

3.7 Definition A quasi-interpolation operator Q is said to provide *polynomial reproduction* of order $m \in \mathbb{N}$ if

$$Q p = p \text{ for all } p \in P^m(\mathbb{R}^d).$$

Following this definition, a suitable result for approximation in fractional Sobolev spaces is given in the literature, to be found in [68, Sect. 3/5]. There, the result is presented in terms of integer Sobolev spaces and Besov spaces, but fractional Sobolev spaces appear as special cases of these (cf. Appendix Sect. 9.2.3ff.).

3.8 Theorem Let $\{Q_h\}_{0 < h < h_0}$ be a family of local quasi-projection operators reproducing P^m on \mathbb{R}^d .

1. Let the basis functions $\{\varphi_i\}_{i \in I}$ satisfy $\|\varphi_i\|_{H^r(\mathbb{R}^d)} \leq b_0^{(1)}$ and $\|\varphi_i^*\|_{L_2(\mathbb{R}^d)} \leq b_0$ for fixed b_0 and some $0 < r < m$. Then we have for $0 < h < h_0$, $0 \leq \varrho < r$ and $F \in H^r(\mathbb{R}^d)$ that

$$\|F - Q_h F\|_{H^\varrho(\mathbb{R}^d)} \leq c h^{r-\varrho} \|F\|_{H^r(\mathbb{R}^d)}.$$

⁽¹⁾The condition on φ_i featured in [68] was actually $\|\varphi_i\|_{B_{p,\infty}^r} \leq b_0$ for Besov space $B_{p,\infty}^r$, but this is clearly implied in our setting by our condition $\|\varphi_i\|_{H^r(\mathbb{R}^d)} \leq b_0$ due to the embedding stated in [96, Sect. 2.3.2].

2. Let the basis functions $\{\varphi_i\}_{i \in I}$ satisfy $\|\varphi_i\|_{H^{m-1}(\mathbb{R}^d)} \leq b_0$ and $\|\varphi_i^*\|_{L_2(\mathbb{R}^d)} \leq b_0$ for fixed $b_0 > 0$. Consider $H^m(\mathbb{R}^d)$. Then we have for $0 < h < h_0$, $\varrho \in [0, m-1]$ and $F \in H^m(\mathbb{R}^d)$ that

$$\|F - Q_h F\|_{H^\varrho(\mathbb{R}^d)} \leq c h^{m-\varrho} \|F\|_{H^m(\mathbb{R}^d)}.$$

Proof: The proof for the first case is given in [68]. The second relation is also given in [68] for \mathbb{R}^d and integer orders, so $\varrho = \mu \in \mathbb{N}_0$. We use the interpolation property from Prop. 2.30 to generalise these to reals: As the relation is valid for integers, we can particularly deduce that the operator norm of $\text{Id} - Q_h$ as an operator from H^m to H^μ for any integer $0 \leq \mu < m$ is $c h^{m-\mu}$. So we have that relation for $\lfloor \varrho \rfloor$ and $\lceil \varrho \rceil$ in particular. Then we obtain with $\theta \in]0, 1[$ and $\varrho = \theta \lfloor \varrho \rfloor + (1 - \theta) \lceil \varrho \rceil$ that

$$\|\text{Id} - Q_h\|_{H^m \rightarrow H^\varrho} \leq c (h^{m-\lfloor \varrho \rfloor})^\theta (h^{m-\lceil \varrho \rceil})^{(1-\theta)} = c h^{m-\theta \lfloor \varrho \rfloor - (1-\theta) \lceil \varrho \rceil} = c h^{m-\varrho}.$$

□

The results of this theorem can be generalised to obtain the same convergence rates also on arbitrary $\Omega \in \text{Lip}_d$ at least theoretically, and there are several options to do so: The first is that for any φ_i such that $\text{supp } \varphi_i(\cdot/h) \cap \Omega \neq \emptyset$ it holds $\text{supp } \varphi_i^*(\cdot/h) \subseteq \Omega$. In this case, the results generalise by definition and we obtain in particular for admissible choices of ϱ

$$\|F - Q_h F\|_{H^\varrho(\Omega)} \leq c h^{r-\varrho} \|F\|_{H^r(\Omega)},$$

and equivalent adaptations of the second statement of the theorem. The second option is that F is actually known in some $\Omega^\sharp \in \text{Lip}_d^*$ such that $\Omega \Subset \Omega^\sharp$. In this case, we can apply the extension operator E_{Ω^\sharp} and obtain $F^\sharp = E_{\Omega^\sharp} F$ that coincides with F on Ω . By the locality property we have then for sufficiently small $h > 0$ that whenever

$$\text{supp } \varphi_i(\cdot/h) \cap \Omega \neq \emptyset \text{ and } \text{supp } \varphi_i^*(\cdot/h) \cap \Omega \neq \emptyset$$

we have also

$$\text{supp } \varphi_i(\cdot/h) \subseteq \Omega^\sharp \text{ and } \text{supp } \varphi_i^*(\cdot/h) \subseteq \Omega^\sharp.$$

In this case, we obtain with the identification of Q_h with $Q_h E_{\Omega^\sharp}$ (that does not affect the result on Ω by locality) for admissible choices of ϱ that

$$\|F - Q_h F\|_{H^\varrho(\Omega)} \leq c h^{r-\varrho} \|F^\sharp\|_{H^r(\Omega^\sharp)}.$$

Again, comparable adaptations of the second statement of the theorem can be deduced similarly. The third option is to define Q_h directly by identifying $Q_h = Q_h E_\Omega$

for the universal continuous extension operator E_Ω . Then we obtain, at least theoretically, for admissible choices of ϱ

$$\|F - Q_h F\|_{H^\varrho(\Omega)} \leq c h^{r-\varrho} \|F\|_{H^r(\Omega)}.$$

As before, we can deduce equivalent adaptations of the second statement of the theorem.

3.9 Remark: These results will prove useful in a two-stage approximation method presented in a later chapter, while we will hardly ever use them otherwise. There, we will be in a situation of a compactly supported objective function, and thus the extension to all of \mathbb{R}^d is easily accomplished.

3.2.2 Interpolating Quasi-Projections

As our final objective in the treatment of general quasi-projection operators, we are now going to investigate if we can enhance them such that $Q_h f$ interpolates f in some finite, fixed set Ξ as long as h is small enough. We will see that we can indeed do so, and this will become very important in future: Once we study approximation in terms of energy functionals in a later chapter, we wish to make use of the convergence orders that quasi-projection operators provide as benchmarks. But sometimes our functionals are only given under strict interpolation constraints, for example if we want to minimise the ESM-equivalent of the energy

$$\int_{\mathbb{R}^d} \sum_{|\alpha|=2} (\partial^\alpha F)^2$$

within the convex set of all functions in $H^2(\mathbb{M})$ that interpolate given function values in a given finite set $\Xi = \{\xi_1, \dots, \xi_n\} \subseteq \mathbb{M}$.

Consequently, our objective is now to determine how such an operator Q_h^Ξ can be constructed at least theoretically to provide us with a benchmark for the "achievable" approximation order. The key ingredient to this is the idea of suitably blending the operator Q_h with an interpolation operator I_h^Ξ in the form

$$Q_h^\Xi := Q_h + I_h^\Xi - I_h^\Xi \cdot Q_h.$$

This idea was for example proposed in [102], and one directly verifies or checks there that $Q_h^\Xi f$ will indeed interpolate a given function f in all $\xi \in \Xi$.

What we still need now is the interpolation operator I_h^Ξ , and we would require it for all $0 < h < h_0$ as long as h_0 is sufficiently small. We will now present a suitable construction method:

First of all, we restrict ourselves to local quasi-projection operators, which will be sufficient for our later treatment. Due to the C^∞ -version of Urysohn's Lemma (cf. [78, Sect. 4.4]), we can find an arbitrarily smooth function $\varphi_\xi : \Omega \rightarrow [0, 1]$ to any $\xi \in \Xi$ that is constantly 1 on $B_{\frac{q_\Xi}{4}}^d(\xi)$ and has support in $B_{\frac{q_\Xi}{2}}^d(\xi)$, where we define as usual the *separation distance* q_Ξ by

$$q_\Xi := \min_{\xi_1, \xi_2 \in \Xi} \|\xi_1 - \xi_2\|_2.$$

Now we define an interpolation operator I_0^Ξ as

$$I_0^\Xi f := \sum_{\xi \in \Xi} f(\xi) \varphi_\xi.$$

Since Ξ *does not* vary when changing h , this function is fixed for any scaling factor h of operator Q_h , and moreover we have for the Sobolev Hilbert space H^r

$$\|I_0^\Xi f\|_{H^r} \leq \max_{\xi \in \Xi} |f(\xi)| \sum_{\xi \in \Xi} \|\varphi_\xi\|_{H^r}.$$

Furthermore, we have as long as $r > \frac{d}{2}$ that $H^r \hookrightarrow C$ by the Sobolev embedding theorem, and we can thereby deduce that

$$\|I_0^\Xi f\|_{H^r} \leq c_\Xi \|f\|_{H^r}.$$

Now we have to choose h_0 small enough such that $Q_h I_0^\Xi f$ is indeed interpolating f at the points of Ξ . That this is actually possible is a consequence of Q being a local quasi-projection operator by assumption and the fact that Ξ is fixed while h can be chosen small: We only have to wait until any basis function and functional for Q_h relevant for the function value at a specific ξ has its whole support contained in $B_{\frac{q_\Xi}{4}}^d(\xi)$. Then if we choose h_0 so small, we obtain that $Q_h I_0^\Xi f$ is interpolating f at any point of Ξ for any $h < h_0$, thereby defining a suitable operator $I_h^\Xi := Q_h I_0^\Xi$. With this operator, we can now define Q_h^Ξ as

$$Q_h^\Xi := Q_h + I_h^\Xi - I_h^\Xi \cdot Q_h.$$

3.10 Remark: It is also worth noting that if Q_h is a projection operator, so $Q_h f = f$ for $f \in F_h$, then Q_h^Ξ is as well a projection operator, as for any $f \in F_h$ it holds

$$Q_h^\Xi f = (Q_h + I_h^\Xi - I_h^\Xi \cdot Q_h) f = Q_h f + I_h^\Xi f - I_h^\Xi f = Q_h f = f.$$

If we are now interested in the approximation power in some space H^r , then we

see that if I_h^Ξ is bounded in the respective space, the approximation power is indeed reproduced:

$$\|f - Q_h^\Xi f\|_{H^r} \leq \|f - Q_h f\|_{H^r} + \|I_h^\Xi f - I_h^\Xi Q_h f\|_{H^r} \leq (1 + \|I_h^\Xi\|_{H^r}) \cdot \|f - Q_h f\|_{H^r}.$$

Taking the construction into account, then I_h^Ξ is bounded at least if Q_h is bounded and if

$$\max_{\xi \in \Xi} |f(\xi)| \sum_{\xi \in \Xi} \|\varphi_\xi\|_{H^r} \leq \max_{\xi \in \Xi} \|\varphi_\xi\|_{H^r} \|f\|_{H^r},$$

with the latter being the case precisely if $H^r \hookrightarrow C$. So we can deduce that orders are reproduced at least whenever $r > \frac{d}{2}$ in our case, which we summarise in the following theorem:

3.11 Theorem *The operator Q_h^Ξ constructed as above from a local quasi-projection operator Q_h for fixed set Ξ reproduces the convergence order of Q_h on H^ϱ whenever Q_h is bounded, $\varrho > \frac{d}{2}$ and $0 < h < h_0$ sufficiently small.*

3.12 Remark: Of course, the $\{\varphi_\xi\}$ need not be from C^∞ to make the above construction work, they only need to be bounded in H^ϱ at least.

3.3 Tensor Product B-Splines

The primary example of an approximation space we are going to revise is that of (uniform) tensor product (B-)splines, in future abbreviated as usual as *TP-splines*. We will employ these as our main technique when it comes to certain other practical applications of our theory, particularly concerning functional minimisations. This is done due to several factors, most importantly:

1. TP-splines have nice approximation properties, particularly when applied in gridded regions. Most importantly, they provide us with suitable operators for quasi-projection operators.
2. There is a considerable number of numerical techniques available that can handle TP-splines, so we can rely on well tested and efficient software packages or components, e.g. in Matlab®.
3. When increasing the number of degrees of freedom, we can rely on the fact that the locality of the basis functions can be increased accordingly without loss of approximation power.

3.3.1 Definition and Initial Approximation Results

Now it is time to give a definition of B-splines as we are going to use them in the subsequent course of this thesis; we restrict ourselves to the case that is commonly known as a *uniform B-spline*, as there seems no real advantage in the application of nonuniform B-splines in the forthcoming chapters — and it simply makes notation and certain other aspects far easier. We follow [89] to define them.

Let $h > 0$ and $m \in \mathbb{N}$. Then we define a function B_1 as

$$B_1(x) := \begin{cases} 1 & -\frac{1}{2} \leq x < \frac{1}{2} \\ 0 & \text{else} \end{cases},$$

and inductively for $m > 1$ the function B_m as

$$B_m(x) := \int_{\mathbb{R}} B_{m-1}(x-t) B_1(t) dt.$$

3.13 Definition Let now $h > 0$ and $n \in \mathbb{Z}$. Then we define the *uniform B-spline* $b_{n,h}^m$ by

$$b_{n,h}^m(x) := B_m\left(\frac{x}{h} + \frac{m}{2} - n\right).$$

For $n \in \mathbb{Z}^d$, the tensor product

$$b_{n,h}^m(x) := b_{n_1,h}^m(x_1) \cdots b_{n_d,h}^m(x_d)$$

of d such B-splines $\{b_{n_j,h}^m(x_j)\}_{j=1}^d$ is called a *tensor product B-spline*. A linear combination s of these basis functions is called a *tensor product spline* and the space of all those splines is denoted by $S_h^m(\mathbb{R}^d)$. If $\Omega \subseteq \mathbb{R}^d$, then the set of all TP-B-splines whose support has nonempty intersection with Ω is called the set of *active B-splines*, and their span is denoted by $S_h^m(\Omega)$.

The set of cells obtained by considering all d -dimensional cubes $C_h(\mathbb{R}^d) := \{c_h[\mathbf{z}] := [0, h]^d + \mathbf{z} : \mathbf{z} \in h \cdot \mathbb{Z}^d\}$ gives all the regions where the restriction of a spline is a polynomial of fixed degree by definition. The subset $C_h(\Omega) \subseteq C_h(\mathbb{R}^d)$ of *active cells* for some $\Omega \subseteq \mathbb{R}^d$ is defined by

$$C_h(\Omega) := \{c \in C_h(\mathbb{R}^d) : c \cap \Omega \neq \emptyset\}.$$

The most important fact for us is that TP-B-splines admit local quasi-projection operators that reproduce P^m . To see this, we make the choice $\varphi_i(\cdot) = b_i^m(\cdot)$ for $i \in \mathbb{Z}^d$ and $h = 1$. Then we start with an initial quasi-projection operator S_1 that

we can explicitly construct. Afterwards, we can go along the lines of Remark 3.6 for scaling to obtain S_h .

We will now determine the initial local quasi-projection operator S_1 by choosing φ_i^* as follows: Since the basis functions are just uniform shifts of $\mathbf{b}_0 = \mathbf{b}_{0,1}$ for the zero vector $\mathbf{0} \in \mathbb{Z}^d$, we fix this $\mathbf{b}_0(x)$ and deduce the general behaviour by shifting. Denote now the other basis functions active on the support of $\mathbf{b}_{0,1}(x)$ by $\mathbf{b}_{\ell^1}, \dots, \mathbf{b}_{\ell^n}$ for suitable $\ell^1, \dots, \ell^n \in \mathbb{Z}^d$. Next, we apply $L_2(\text{supp } \mathbf{b}_0)$ -Gram-Schmidt orthogonalisation to the sequence $\mathbf{b}_{\ell^1}, \dots, \mathbf{b}_{\ell^n}, \mathbf{b}_0$ in that order to obtain mutually orthogonal $\tilde{\mathbf{b}}_{\ell^1}, \dots, \tilde{\mathbf{b}}_{\ell^n}, \tilde{\mathbf{b}}_0$. The resulting $\tilde{\mathbf{b}}_0$ is now our choice for the dual function, but we still have to justify that this choice is valid:

First of all, one can directly see that the support of $\tilde{\mathbf{b}}_0$ is bounded, and that by construction $\tilde{\mathbf{b}}_0$ is L_2 -orthogonal to the initial $\mathbf{b}_{\ell^1}, \dots, \mathbf{b}_{\ell^n}$, as

$$\text{span}\{\mathbf{b}_{\ell^1}, \dots, \mathbf{b}_{\ell^n}\} = \text{span}\{\tilde{\mathbf{b}}_{\ell^1}, \dots, \tilde{\mathbf{b}}_{\ell^n}\} \perp \tilde{\mathbf{b}}_0.$$

The resulting operator Λ_0 is then defined by

$$\Lambda_0 f = \int_{\text{supp } \mathbf{b}_0} f \cdot \tilde{\mathbf{b}}_0,$$

and it is bounded on L_p , as by Hölder's inequality

$$\int_{\text{supp } \mathbf{b}_0} f \cdot \tilde{\mathbf{b}}_0 \leq \|f\|_{L_p(\text{supp } \mathbf{b}_0)} \cdot \|\tilde{\mathbf{b}}_0\|_{L_{p^*}(\text{supp } \mathbf{b}_0)}.$$

Suitable rescaling of $\tilde{\mathbf{b}}_0$ gives $\int \tilde{\mathbf{b}}_0 \cdot \mathbf{b}_0 = 1$ without any harm. Since the basis function \mathbf{b}_0 was chosen arbitrarily, this construction will do for any B-spline by simple translation of our given functional. Then we define the functionals $\{\Lambda_{n,h}\}_{n \in \mathbb{Z}}$ for arbitrary h and S_h^m as proposed in Remark 3.6 by appropriate scaling. Simple calculation and application of the transformation law shows then that the operator norms of S_h and S_1 for L_p coincide.

Furthermore, the resulting operator is a true projector onto S_h^m and thus provides reproduction of polynomials in particular: This can directly be deduced from the fact that any functional reproduces the corresponding basis function by construction, and so in particular any polynomial of total order at most m is reproduced, as we clearly have $P^m(\mathbb{R}^d) \subseteq S_h^m(\mathbb{R}^d)$. In fact, even tensor product polynomials of order at most m are reproduced by the same argument.

3.14 Remark: (1) When it comes to practical implementation, it is convenient to see that in case $p = 2$ the above process gives us Λ_0 as the value β_{ℓ^0} for $\ell^0 = \mathbf{0}$ obtained from the quadratic minimisation problem

$$\int_{\text{supp } \mathbf{b}_0} \left(\sum_{i=0}^n \beta_{\ell^i} \mathbf{b}_{\ell^i} - f \right)^2 \rightarrow \min!$$

This holds because the ONB gives a projection operator in this Hilbert space case, and then the two definitions of the functional turn out to be effectively equal.

(2) One can also perform the prescribed projection / minimisation separately on each cell of the support, and take the average of the results as the ultimate choice for the coefficient. Theoretically, this results in m^d independent quasi-projections, namely one for each fixed cell position in a support, whose average is taken afterwards, but all relevant properties remain unaffected. Similarly, one could also use arbitrary suitable subsets of $\text{supp } \mathbf{b}_0$, in particular just a single cell.

Since we have now defined suitable local quasi-projections (even projections), we can in particular deduce that the results of Theorem 3.8 hold for TP-splines. However, still undetermined in this context remains the exact regularity of a TP-B-spline in the Hilbert Sobolev sense. Clearly, any such B-spline is in H^{m-1} , but the question is whether we can obtain actually $H^{m-\delta}$ for some $0 < \delta < 1$. The answer is indeed affirmative for $\delta > \frac{1}{2}$, but we need the definition of Besov spaces in terms of moduli of smoothness for this, which we briefly revised in the appendix: By example 9.13 presented there, we obtain that a univariate uniform B-spline is in $H^{m-\frac{1}{2}-\varepsilon}$ for any $\varepsilon > 0$. Consequently, a multivariate TP-B-spline is therefore as well at least in $H^{m-\frac{1}{2}-\varepsilon}$ — we can deduce this directly by Fubini. So the supremal choice for r in the first statement of Theorem 3.8 is $m - \frac{1}{2}$.

3.15 Corollary *Let $\{S_h\}_{0 < h < h_0}$ be a family of local quasi-projection operators on $S_h^m(\mathbb{R}^d)$ as introduced above. Then the results of Theorem 3.8 are applicable. Therein, the supremum of the admissible choices for $r > 0$ in the first statement is at least $m - \frac{1}{2}$.*

3.3.2 Locality of Approximation and the Continuity of Operators

We proceed with some more elaborate considerations on the local approximation power of local quasi-interpolants based on splines, using [89, §12.3, §13.3, §13.4]:

3.16 Lemma *Let $1 \leq p < \infty$ and $0 < n \leq m \in \mathbb{N}$. Let $c_h[\mathbf{z}]$ be an arbitrary cell for the spline space $S_h^m(\mathbb{R}^d)$, and $\xi \in c_h[\mathbf{z}]$ and $f \in W_p^n(B_{mh}[\mathbf{z}])$. Let further $0 \leq \mu < n$ and let $T_{n,\xi}$ be the averaged Taylor polynomial of (tensorial or total) maximal order n to f in ξ . Then holds the relation*

$$\|f - T_{n,\xi}\|_{W_p^\mu(c_h[\mathbf{z}])} \leq \|f - T_{n,\xi}\|_{W_p^\mu(B_{mh}[\mathbf{z}])} \leq c h^{n-\mu} \|f\|_{W_p^n(B_{mh}[\mathbf{z}])}.$$

Proof: This is just (averaged) Taylor remainder estimation due to [89, §13.4]. \square

3.17 Lemma *In the setting of the last lemma, any local quasi-projection operator S_h reproducing polynomials of order m will satisfy*

$$\|f - S_h f\|_{W_p^\mu(c_h[z])} \leq c \|f - T_{n,\xi}\|_{W_p^\mu(B_{mh}[z])} \leq c h^{n-\mu} \|f\|_{W_p^n(B_{mh}[z])}.$$

If furthermore $n < m$, then it holds even

$$\|f - S_h f\|_{W_p^n(c_h[z])} \leq c \|f\|_{W_p^n(B_{mh}[z])}.$$

Proof: The first claim can be deduced from the last lemma by polynomial reproduction properties of S_h via

$$\begin{aligned} \|f - S_h f\|_{W_p^\mu(c[z])} &\leq \|f - T_{n,\xi}\|_{W_p^\mu(c[z])} + \|T_{n,\xi} - S_h f\|_{W_p^\mu(c[z])} \\ &= \|f - T_{n,\xi}\|_{W_p^\mu(c[z])} + \|S_h T_{n,\xi} - S_h f\|_{W_p^\mu(c[z])}. \end{aligned}$$

There, the first summand is bounded by $c h^{n-\mu} \|f\|_{W_p^n(B_{mh}[z])}$ for any $\mu < n$, but the second will need some arguments: We take for an arbitrary suitable ordering and appropriate index set I_* the basis functions $\{b_{\ell^i}^m\}_{i \in I_*}$ and functionals $\{\Lambda_{\ell^i, h}\}_{i \in I_*}$ of S_h active on $c[z]$. Then we obtain for $R = f - T_{n,\xi}$ by the triangle inequality

$$\|S_h R\|_{W_p^\mu(c[z])} \leq \sum_{i \in I_*} |\Lambda_{\ell^i, h} R| \cdot \|b_{\ell^i}^m\|_{W_p^\mu(c[z])}.$$

We can bound $\|b_{\ell^i}^m\|_{W_p^\mu(c[z])}$ by $c \cdot h^{-\mu}$ due to the chain rule and the construction of the $b_{\ell^i}^m$ by scaling and shifting. By continuity and locality of the $\Lambda_{\ell^i, h}$, we obtain

$$|\Lambda_{\ell^i, h} R| \leq c \|f - T_{n,\xi}\|_{L_p(\text{supp } b_{\ell^i}^m)} \leq c \|f - T_{n,\xi}\|_{L_p(B_{mh}[z])} \leq c h^n \|f\|_{W_p^n(B_{mh}[z])},$$

which finishes the first claim by insertion. For proving the second claim, we suppose the order of the Taylor polynomial to be total and observe that it still holds

$$\|f - S_h f\|_{W_p^n(c[z])} \leq \|f - T_{n,\xi}\|_{W_p^n(c[z])} + \|S_h T_{n,\xi} - S_h f\|_{W_p^n(c[z])}.$$

Now the first summand satisfies due to totality of the order the relation $D^n T_{n,\xi} = 0$, and so we can deduce that

$$\|f - T_{n,\xi}\|_{W_p^n(c[z])} \leq \|f - T_{n,\xi}\|_{W_p^{n-1}(c[z])} + \|f\|_{W_p^n(c[z])},$$

where the right hand side can be bounded by $c \|f\|_{W_p^n(B_{mh}[z])}$. And for the second term we can just proceed as in case $\mu < n$, because in particular $\|b_\ell^m\|_{W_p^n(c[z])}$ is still well-defined as we are in the situation $n < m$. \square

As a direct consequence of this lemma, the approximation power of the operator S_h is clearly localised. So if we take all cells that are active on $U_{ah}(\mathbb{M})$ for some $a > 0$ and \mathbb{M} without boundary, then because of the finite, globally bounded overlap of the $B_{mh}[z]$ for all relevant cell bases z to cells in $C_h(U_{ah}(\mathbb{M}))$ we conclude after summing over all cells for sufficiently small h

$$\begin{aligned} \|F - S_h F\|_{W_p^\mu(U_{ah})} &\leq \sum_{c[z] \in C_h(U_{ah})} \|F - S_h F\|_{W_p^\mu(c[z])} \\ &\leq c h^{m-\mu} \sum_{c[z] \in C_h(U_{ah})} \|F\|_{W_p^\mu(B_{mh}[z])} \leq c h^{m-\mu} \|F\|_{W_p^m(U_{bh})} \end{aligned}$$

with suitable $b > a + d(m+1)$. Consequently, we obtain that S_h is an approximation operator that is local relative to \mathbb{M} , and we can transfer the results of Theorem 3.3:

3.18 Corollary *Let in the general setting of Theorem 3.3 $\mathbb{M} \in \mathbb{M}_{\text{cp}}^k(\mathbb{R}^d)$ and $\{S_h\}_{0 < h < h_0}$ be a family of local spline quasi-projection operators on $S_h^m(U(\mathbb{M}))$ reproducing P^m . Let $0 < n \leq m$ and $0 \leq \mu \leq n - \kappa$ be such that $\mu < m - \kappa$. Then we have for $S_h^N := T_{\mathbb{M}} S_h E_N$ and any $f \in W_p^n(\mathbb{M})$ the relation*

$$\|f - S_h^N f\|_{W_p^\mu(\mathbb{M})} \leq c h^{n-\mu} \|f\|_{W_p^n(\mathbb{M})}.$$

3.19 Remark: (1) If \mathbb{M} has a boundary, then the same holds at least for $S_h^N := R_{\mathbb{M}} T_{\widehat{\mathbb{M}}} S_h E_N E_{\widehat{\mathbb{M}}}^{\widehat{\mathbb{M}}}$, where $E_{\widehat{\mathbb{M}}}^{\widehat{\mathbb{M}}}$ is the continuous extension operator that maps $W_p^n(\mathbb{M})$ to $W_p^n(\widehat{\mathbb{M}})$ for $\widehat{\mathbb{M}} \in \mathbb{M}_{\text{cp}}^k(\mathbb{R}^d)$ without boundary such that $\mathbb{M} \Subset \widehat{\mathbb{M}}$ we have required to exist. The impact of this result for \mathbb{M} with boundary is again of rather theoretical interest, but still useful in estimating the theoretically achievable approximation order in that case.

(2) Despite the notorious problem of approximation in arbitrary domains with splines, a suitable practicable definition of the approximation operator also in the case with boundary is not beyond reach, as arguments in [79] imply.

3.20 Remark: In the case $p = \infty$, which we neglected in the whole thesis, the above result is also valid, as can be found in [82] exemplarily discussed for TP-splines. There, it is also stated that actually for all $1 \leq \mu < m-1$ and any $f \in W_\infty^m(\mathbb{M})$ it holds

$$\|f - S_h^N f\|_{W_\infty^\mu(\mathbb{M})} \leq c h^{m-\mu} \|f\|_{W_\infty^m(\mathbb{M})}.$$

We will see soon that for extensions based on a *linear* foliation we can also achieve $1 \leq \mu < m$ even in case $p < \infty$.

In addition to this, we obtain also a result on continuity of local quasi-projection operators not only on Lebesgue but also on higher and fractional order Sobolev spaces. On the one hand, we can deduce suitable interpolating quasi-projection operators thereby, and on the other hand it gives us a handle to deduce

$$\|f - S_h f\|_{H^\varrho} \leq c \|f\|_{H^\varrho}$$

for the limiting case $f \in H^\varrho$.

3.21 Theorem *Let $\{S_h\}_{0 < h < h_0}$ be a family of local spline quasi-projection operators on $S_h^m(\mathbb{R}^d)$ as introduced above. Then S_h is a bounded operator on $W_p^\mu(\mathbb{R}^d)$ whenever $0 \leq \mu \leq m - 1$ ($\mu \in \mathbb{N}_0$) and on $H^\varrho(\mathbb{R}^d)$ whenever $0 \leq \varrho \leq m - 1$. The same relation holds on any $\Omega \in \text{Lip}_d$ for S_h^Ω defined by $S_h^\Omega = R_\Omega S_h E_\Omega$ and $W_p^\mu(\Omega)$ resp. $H^\varrho(\Omega)$.*

Proof: Due to the finite, globally bounded overlap of any collection of balls $B_{mh}[z]$ as in Lemma 3.17, the last statement of that lemma and the triangle inequality, the claim is clear for any $W_p^\mu(\mathbb{R}^d)$ with $0 \leq \mu \leq m - 1$. Then the relation for noninteger spaces on \mathbb{R}^d follows by interpolation of operator norms in the interpolation property of Prop. 2.30: We choose $m_1 = n_1 = \lfloor \varrho \rfloor$, $m_2 = n_2 = \lceil \varrho \rceil$ and $0 < \theta < 1$ such that $\varrho = \theta m_1 + (1 - \theta)m_2$ and insert in Prop. 2.30.

In all cases, the relation for $\Omega \in \text{Lip}_d$ is a consequence of the respective result for, applied to the bounded extension from Ω to \mathbb{R}^d if the function is not initially known on all of \mathbb{R}^d . \square

3.22 Remark: Note in particular that due to boundedness of S_h^Ω in any W_p^n with $n < m$ we have that for any $f \in W_p^n(\Omega)$

$$\|f - S_h^\Omega f\|_{W_p^n(\Omega)} \leq c \|f\|_{W_p^n(\Omega)}.$$

This gives us a key for handling functions of limited regularity with splines of higher orders. In particular, we have that approximations of functions in H^2 are bounded by a constant factor times the initial function norm whenever $m > 2$, so in literally any situation where considering second derivatives of the splines makes sense.

One further consequence of this result is that we can enhance the validity of Theorem 3.8 for TP-splines, and thus Cor. 3.15, in the following way:

3.23 Corollary *Let $\{S_h\}_{0 < h < h_0}$ be a family of local spline quasi-projection operators for $S_h^m(\mathbb{R}^d)$ reproducing P^m . Consider $H^r(\mathbb{R}^d)$ and arbitrary $0 \leq r \leq m$. Then we have for $0 < h < h_0$ and $\varrho \leq \min(\lfloor r \rfloor, m - 1)$ that*

$$\|F - S_h F\|_{H^\varrho(\mathbb{R}^d)} \leq c h^{r-\varrho} \|F\|_{H^r(\mathbb{R}^d)}.$$

Proof: By the last theorem, we have in particular that for any $0 \leq \mu \leq \min(n, m-1)$ and arbitrary fixed $n \leq m$

$$\|F - S_h F\|_{H^\mu(\mathbb{R}^d)} \leq c h^{n-\mu} \|F\|_{H^n(\mathbb{R}^d)}.$$

We can easily deduce that for any real $0 \leq \varrho \leq \min(n, m-1)$

$$\|F - S_h F\|_{H^\varrho(\mathbb{R}^d)} \leq c h^{n-\varrho} \|F\|_{H^n(\mathbb{R}^d)}. \quad (3.23.1)$$

This comes by interpolation as applied in the proof of 3.8. Now we have to apply the interpolation property from Prop. 2.30 in a second step once again. So we choose first some real, noninteger $r < m$. We can choose $\varrho \leq m_1 < m_2 \leq m$ and $0 < \theta < 1$ such that $r = \theta m_1 + (1-\theta)m_2$, e. g. $m_1 = \lfloor r \rfloor$ and $m_2 = \lceil r \rceil$. If we now apply the interpolation property for $\varrho_1 = \varrho_2 = \varrho$, we obtain by virtue of (3.23.1) for the operator $\text{Id} - S_h$ that

$$\|F - S_h F\|_{H^\varrho(\mathbb{R}^d)} \leq c h^{\theta(m_1-\varrho)+(1-\theta)(m_2-\varrho)} \|F\|_{H^r(\mathbb{R}^d)}.$$

This is already the desired result. □

3.24 Remark: Note that this corollary is *not* equivalent to the first statement in 3.8 for TP-splines. There, by the regularity of splines, the supremum of admissible choices for r was $m - \frac{1}{2}$, while any $\varrho < r$ could be chosen. In contrast to this, we can have any $r \leq m$ here but must have $\varrho \leq \min(\lfloor r \rfloor, m-1)$.

3.3.3 Improved Approximation Results

In Theorem 3.3 and its TP-spline version in Corollary 3.18, the range for μ is rather restricted when it comes to higher codimensions. Consequently, we would hope for an improvement. Of course, this improvement comes not for free: While any of the previous results would remain valid if we would replace E_N by some other E_F for an arbitrary M-foliation F , in the following this foliation would need to be linear — but still, our normal foliation and extension can remain the rolemodel, as these are obviously linear.

Before we come to the actual statement and proof, we will have to make some additional auxiliary statements within a couple of lemmas:

3.25 Lemma *Let $\varphi : \Omega \rightarrow \Omega_\varphi$ be a bidirectionally C-bounded smooth diffeomorphism. Then there are $a_1, a_2, b_1, b_2 > 0$ such that we have for any $y \in \Omega$, $x = \varphi(y)$ and any $r_0 > r > 0$ the relations*

$$\begin{aligned}\varphi(B_{a_1 r}(y)) &\subseteq B_r(x) \subseteq \varphi(B_{a_2 r}(y)), \\ \varphi^{-1}(B_{b_1 r}(x)) &\subseteq B_r(y) \subseteq \varphi^{-1}(B_{b_2 r}(x)).\end{aligned}$$

The same relations hold (with possibly other constants) if one replaces the Euclidean norm ball $B(\cdot)$ by the maximum norm ball $B[\cdot]$.

Proof: Due to equivalence of norms, it suffices to give the respective result just for the Euclidean norm balls. There we have for arbitrary $z \in B_r(x)$ by the mean value theorem for some convex combination ξ of x and z that

$$\begin{aligned}\|\varphi^{-1}(z) - \varphi^{-1}(x)\|_2 &= \|D\varphi^{-1}(\xi)(z - x) + \varphi^{-1}(x) - \varphi^{-1}(x)\|_2 \\ &\leq \max_{w \in \Omega_\varphi} \|(D\varphi^{-1}(w))_{ij}\|_2 \cdot \|z - x\|_2\end{aligned}$$

which is globally bounded from above by $c\|x - z\|_2$ for φ being bidirectionally C-bounded. In the same way, we obtain the other relations. \square

Using this, we can now give the following result on containment of images and preimages of balls in parameter spaces:

3.26 Lemma *Let $M \in \mathbb{M}_{\text{cp}}^k(\mathbb{R}^d)$ and $U_\varepsilon(M)$ have the closest point property. Let both be parameterised according to inverse atlases $A_M \in \mathbb{I}(M)$ and $U_M \in \mathbb{I}_N^{\text{ex}}(M)$, respectively. Let further $\delta > 0$ be given. Then we can choose $0 < a < b < \infty$, some $h_0 > 0$ and the inverse atlases A_M of M and U_M of $U_\varepsilon(M)$ in such a way that it holds for any $0 < h < h_0$ and any $x \in U_{ah}(M)$*

- *the closure of the ball $B_{h\delta}[x]$ is contained in $U_{hb}(M)$,*
- *there is $(\Psi, \Omega) \in U_M$ such that $\Psi^{-1}(B_{h\delta}[x]) \subseteq \Omega$.*

Proof: The first statement is fairly obvious: We simply have to demand h_0 is so small that we can choose $b > a + d\delta$ and $U_{bh_0}(M)$ has the closest point property. The second statement requires slightly more considerations: By our choice of $(\psi_i, \omega_i)_{i \in I} \in \mathbb{I}(M)$ and compactness, we see that there is some fixed $\varrho > 0$ such that not only the collection $(\psi_i, \omega_i)_{i \in I}$ parameterises M , but also $(\psi_i, \omega_i^\#)_{i \in I}$ for suitable

$$\omega_i^\# \subseteq \{z \in \omega_i : \|z - \partial\omega_i\|_\infty > \varrho\}.$$

As we can always rely on cylinders or balls for the parameter spaces, we can therein obviously choose again Lipschitz sets. Then for an arbitrary $x \in U_{ah}(M)$, there is some suitable $(\psi_j, \omega_j^\#)$ such that $x \in \Psi(\omega_j^\# \times B_{ah}^k(0))$. Thereby we can deduce by the previous Lemma 3.25 that with h_0 sufficiently small it holds

$$\Psi^{-1}(B_{h\delta}[x]) \subseteq B_{h\delta\tilde{a}}[\Psi^{-1}(x)] \subseteq \omega_j \times B_{ah}^\kappa(0)$$

for some fixed $\tilde{a} > 0$, which gives the desired relation. \square

3.27 Lemma *Let P be a polynomial of (tensorial or total) order at most $m \in \mathbb{N}$. Let $\Omega \subseteq \mathbb{R}^d$ be compact and $0 < a < b$. Then there is a constant $c > 0$ that depends only on m, a, b, q such that it holds for any $r > 0$ and $x \in \Omega$*

$$\int_{B_{br}[x]} (P(z-x))^q dz \leq c \int_{B_{ar}[x]} (P(z-x))^q dz.$$

Proof: We suppose the polynomial to be in Taylor form with center x and thus can restrict ourselves to $x = 0$ now; all other positions then come by translation. We first consider the case of P being a monomial, so $P_\alpha(z) := z^\alpha$ with $|\alpha_j| < m$ for all $j = 1, \dots, d$. Now we transform $B_{br}[0]$ and $B_{ar}[0]$ to the unit square and obtain

$$\begin{aligned} \int_{B_{br}[0]} (P_\alpha(z))^q &= \int_{B_1[0]} (P_\alpha(rb \cdot z))^q (br)^d = b^{d+q \cdot |\alpha|} r^{d+q \cdot |\alpha|} \int_{B_1[0]} (P_\alpha(z))^q, \\ \int_{B_{ar}[0]} (P_\alpha(z))^q &= \int_{B_1[0]} (P_\alpha(ra \cdot z))^q (ar)^d = a^{d+q \cdot |\alpha|} r^{d+q \cdot |\alpha|} \int_{B_1[0]} (P_\alpha(z))^q. \end{aligned}$$

Hence we conclude

$$\|P_\alpha\|_{L_q(B_{ar}[0])}^q \leq \|P_\alpha\|_{L_q(B_{br}[0])}^q \leq (b/a)^{(d+m \cdot d)} \|P_\alpha\|_{L_q(B_{ar}[0])}^q,$$

and choose the desired constant as $c_{a,b} = (b/a)^{d(m+1)}$. This constant will then suffice for any monomial. To deal with the general case, we demand that

$$P(z) = \sum_{\substack{\alpha \in \mathbb{N}_0^d \\ |\alpha_j| < m}} c_\alpha z^\alpha.$$

By equivalence of norms in finite dimensional spaces, we have for any such polynomial

$$\sum_{\substack{\alpha \in \mathbb{N}_0^d \\ |\alpha_j| < m}} |c_\alpha| \cdot \|P_\alpha\|_{L_q(B_a[0])} \leq c \|P\|_{L_q(B_a[0])}. \quad (3.27.1)$$

We wish to achieve for a constant independent of $r > 0$ that

$$\sum_{\substack{\alpha \in \mathbb{N}_0^d \\ |\alpha_j| < m}} |c_\alpha| \cdot \|P_\alpha\|_{L_q(B_{ar}[0])} \leq c \|P\|_{L_q(B_{ar}[0])}, \quad (3.27.2)$$

as this would allow us to conclude by the triangle inequality

$$\|P\|_{L_q(B_{br}[0])} \leq \sum_{\substack{\alpha \in \mathbb{N}_0^d \\ |\alpha_j| < m}} |c_\alpha| \cdot \|P_\alpha\|_{L_q(B_{br}[0])} \leq c_{a,b} \sum_{\substack{\alpha \in \mathbb{N}_0^d \\ |\alpha_j| < m}} |c_\alpha| \cdot \|P_\alpha\|_{L_q(B_{ar}[0])} \leq c \|P\|_{L_q(B_{ar}[0])}.$$

By the transformation law we have for any polynomial P and any $r > 0$

$$\|P(\cdot)\|_{L_q(B_{ra}[0])} = r^{d/q} \|P(r\cdot)\|_{L_q(B_a[0])}.$$

As any $r^{d/q}$ would appear on both sides and thus would cancel out in (3.27.2), it suffices for (3.27.2) to prove that it holds

$$\sum_{\substack{\alpha \in \mathbb{N}_0^d \\ |\alpha_j| < m}} |c_\alpha| \cdot \|P_\alpha(r\cdot)\|_{L_q(B_a[0])} \leq c \|P(r\cdot)\|_{L_q(B_a[0])}.$$

If we now take a look at $c_\alpha P_\alpha(r\cdot)$, we see that

$$c_\alpha P_\alpha(r\cdot) = c_\alpha r^\alpha P_\alpha(\cdot).$$

Consequently, we can assign new coefficients $c_\alpha(r) := c_\alpha r^\alpha$ and reduce the inequality to

$$\sum_{\alpha} |c_\alpha(r)| \cdot \|P_\alpha(\cdot)\|_{L_q(B_a[0])} \leq c \sum_{\alpha} c_\alpha(r) P_\alpha(\cdot) \|_{L_q(B_a[0])}.$$

But with these new coefficients, this is precisely (3.27.1), which we know is true for *any* choice of coefficients with a constant independent of these. \square

3.28 Lemma *Let P_f be the polynomial that coincides with $S_h f$ for fixed $f \in W_q^m(\mathbb{R}^d)$ on some arbitrary cell $c_h[\mathbf{z}] = B_{h/2}[\zeta]$. Then we have for any $0 \leq \mu < m$, any fixed $b \geq \varepsilon > 0$ and sufficiently small $0 < h < h_0$ the relation*

$$\|f - P_f\|_{W_q^\mu(B_{bh}[\zeta])} \leq c h^{m-\mu} \|f\|_{W_q^\mu(B_{mbh}[\zeta])}.$$

Proof: We see that by Taylor remainder estimation for T_f the averaged Taylor polynomial of (tensorial or total) order m to f in ζ , and by the previous result with $a = \frac{1}{2}$ that

$$\begin{aligned} \|f - P_f\|_{W_q^\mu(B_{bh}[\zeta])} &\leq \|f - T_f\|_{W_q^\mu(B_{bh}[\zeta])} + \|P_f - T_f\|_{W_q^\mu(B_{bh}[\zeta])} \\ &\leq c h^{m-\mu} \|f\|_{W_q^\mu(B_{mbh}[\zeta])} + c \|P_f - T_f\|_{W_q^\mu(B_{h/2}[\zeta])}. \end{aligned}$$

The second summand can now be dealt with due to quasi-projection properties as in the proof of Lemma 3.17 to obtain

$$\begin{aligned}\|P_f - T_f\|_{W_q^\mu(B_{h/2}[\zeta])} &= \|S_h f - S_h T_f\|_{W_q^\mu(B_{h/2}[\zeta])} \leq c h^{m-\mu} \|f\|_{W_q^\mu(B_{mh}[\zeta])} \\ &\leq c h^{m-\mu} \|f\|_{W_q^\mu(B_{mbh}[\zeta])}.\end{aligned}$$

□

Now we have assembled everything we need to improve the results of Theorem 3.3 in case of TP-splines and a linear foliation:

3.29 Theorem *Let $M \in \mathbb{M}_{\text{cp}}^k(\mathbb{R}^d)$. Let $\{S_h\}_{0 < h < h_0}$ be a family of local spline quasi-projection operators on $S_h^m(U(M))$ reproducing P^m . Let $1 < q < \infty$, $0 < n \leq m$ and let $0 \leq \mu \leq n - 1$ be such that $\mu < m - 1$. Define $S_h^N := T_M S_h E_N$. Then we have for any $f \in W_q^n(M)$ the relation*

$$\|f - S_h^N f\|_{W_q^\mu(M)} \leq c h^{n-\mu} \|f\|_{W_q^n(M)}.$$

Proof: In the proof, we are heading for application of the previous lemma, so we have to check for the requirements and its applicability. Let $\{c_h(z)\}_{z \in Z_{a,h}} = \{c_h(\zeta - h/2 \cdot \mathbf{1})\}^{(2)}$ be the set of cells of length h that make up $C_h(U_{ah}(M))$. The points ζ with $\zeta - h/2 \cdot \mathbf{1} \in Z_{a,h} \subseteq h\mathbb{Z}$ make up the centers of the cells, so that each cell has the form $B_{h/2}[\zeta]$. Without restriction, we demand $a < 1/(2d)$ in Lemma 3.27. Let $S_h = S_h \vec{F}$ for $\vec{F} = E_N f$ on these cells and let s_h be its trace on M . Let c_h be an arbitrary cell seen as an axis aligned cube $B_{h/2}[\zeta]$ with center ζ . Then $(S_h)_{|c_h} = P_{c_h}$ for some polynomial P_{c_h} of order m , and we name by $p_{c_h} = T_M P_{c_h}$ the trace on all of M for P_{c_h} considered as a polynomial on \mathbb{R}^d . Because any cell $B_{h/2}[\zeta]$ is compactly contained in $B_h[\zeta]$, we have that

$$\|f - s_h\|_{W_q^\mu(M)} \leq c \sum_{\zeta \in Z_{a,h}} \|f - p_{c_h}\|_{W_q^\mu(M \cap B_h[\zeta])}.$$

We have by Lemmas 3.25 and 3.26 that for sufficiently small $h > 0$ to any $B_h[\zeta]$ there is an appropriate pair $(\Psi, \Omega) = (\Psi(c_h), \Omega(c_h))$ such that the preimage of $B_h[\zeta]$ is compactly contained in Ω , and we restrict ourselves to this Ω and Ψ for the further treatment of $W_q^\mu(M \cap B_h[\zeta])$. We are now going to bound $\|f - p_{c_h}\|_{W_q^\mu(M \cap B_h[\zeta])}$ suitably: By Lemmas 3.25 and 3.26, we even have for $\xi = \Psi^{-1}(\zeta)$ and some constant $c_1 > 0$ valid over the whole inverse atlas as long as h is sufficiently small

$$\Psi^{-1}(B_h[\zeta]) \subseteq B_{c_1 h}[\xi] \Subset \Omega.$$

Now we abbreviate $P = P_{c_h}$, $p = p_{c_h}$ and $\vec{P} = E_N p$. We are then going to prove that for \tilde{b} independent of f, P, ζ :

⁽²⁾ $\mathbf{1}$ is the all-one vector in \mathbb{R}^d

$$\|f - p\|_{W_q^\mu(B_h[\zeta] \cap M)} \leq c h^{n-\mu-\kappa/q} \|\vec{F}\|_{W_q^n(B_{bh}[\zeta])}.$$

Because we have $\Psi^{-1}(B_h[\zeta]) \subseteq B_{c_1 h}[\xi]$ for some fixed c_1 , we have that

$$\|f - p\|_{W_q^\mu(B_h[\zeta] \cap M)}^q \leq c \sum_{|\alpha| \leq \mu} \int_{\omega \cap B_{c_1 h}[\xi]} (\partial^\alpha (f \circ \psi - p \circ \psi))^q.$$

Therein, we have used implicitly that if $\omega \cap B_{c_1 h}[\xi] \subseteq \omega$ it holds for the collection $\{(\psi_{\zeta,j}, \omega_{\zeta,j})\}_{j=1}^\ell \subseteq \mathbb{A}_M$ that satisfies $\psi_{\zeta,j}(\omega_{\zeta,j}) \cap B_h[\zeta] \neq \emptyset$ the additional relation

$$\sum_{1 \leq j \leq \ell} \sum_{|\eta| \leq \mu} \int_{\psi_{\zeta,j}^{-1}(B_h[\zeta] \cap M)} (\partial^\eta (f \circ \psi_{\zeta,j} - p \circ \psi_{\zeta,j}))^q \leq c \sum_{|\alpha| \leq \mu} \int_{\omega \cap B_{c_1 h}[\xi]} (\partial^\alpha (f \circ \psi - p \circ \psi))^q$$

for a constant independent of f , but we can require this by construction of our inverse atlas. Now we take an arbitrary multi-index $\alpha = (\alpha_{\underline{k}}, \alpha_{\underline{\kappa}})$ with $|\alpha| \leq \mu < m - 1$, where $\alpha_{\underline{k}}$ consists of the first k and $\alpha_{\underline{\kappa}}$ of the last κ entries of α , and define consequently $\partial^\alpha = \partial_{x^{\underline{k}}}^{\alpha_{\underline{k}}} \partial_{z^{\underline{\kappa}}}^{\alpha_{\underline{\kappa}}}$. Using the equivalence of norms defined on ω and on Ω for constant extension by E_N due to Theorem 2.26, we obtain

$$\begin{aligned} \int_{\omega \cap B_{c_1 h}[\xi]} (\partial^\alpha (f \circ \psi - p \circ \psi))^q &\leq c h^{-\kappa} \int_{B_{c_1 h}[\xi]} (\partial^\alpha (\vec{F} \circ \Psi - \vec{P} \circ \Psi))^q \\ &\leq c h^{-\kappa} \int_{B_{c_1 h}[\xi]} (\partial^\alpha (\vec{F} \circ \Psi - P \circ \Psi))^q + c h^{-\kappa} \int_{B_{c_1 h}[\xi]} (\partial^\alpha (\vec{P} \circ \Psi) - P \circ \Psi)^q. \end{aligned} \quad (3.29.1)$$

We start with the first summand, where we have with norm equivalence under diffeomorphisms, the C-boundedness of Ψ as applied before, Lemma 3.25 for a suitable $c_2 > 0$ and the approximation assumptions on P due to Lemma 3.28

$$\begin{aligned} \int_{B_{c_1 h}[\xi]} (\partial^\alpha (\vec{F} \circ \Psi - P \circ \Psi))^q &\leq c \int_{\Psi(B_{c_1 h}[\xi])} \sum_{|\beta| \leq |\alpha|} (\partial^\beta (\vec{F} - P))^q \\ &\leq c \int_{B_{c_2 h}[\zeta]} \sum_{|\beta| \leq |\alpha|} (\partial^\beta (\vec{F} - P))^q \\ &\leq c h^{q(n-|\alpha|)} \|\vec{F}\|_{W_q^n(B_{mc_2 h}[\zeta])}^q. \end{aligned} \quad (3.29.2)$$

Therein we ensure $h < h_0$ is so small that $B_{mc_2 h}[\zeta] \subseteq \Psi(\Omega)$, possibly restricting h_0 further. Now we have arrived at our goal with the first summand of (3.29.1), as with $\tilde{b} \geq m c_2$ clearly

$$\|\vec{F}\|_{W_q^n(B_{mc_2 h}[\zeta])}^q \leq \|\vec{F}\|_{W_q^n(B_{bh}[\zeta])}^q.$$

Turning to the second summand, we use $B_{c_3 h}^\omega[\xi] := B_{c_3 h}[\Pi_\omega(\xi)] \cap \omega$ for suitable $c_3 \geq c_1$ such that $B_{c_1 h}[\xi] \subseteq B_{c_3 h}[\Pi_\omega(\xi)]$. Then we distinguish the two cases $|\alpha_{\underline{k}}| = 0$ and $|\alpha_{\underline{k}}| > 0$ again, as we did in the proof of Theorem 3.3: In case $|\alpha| = |\alpha_{\underline{k}}|$

we observe that because the normal foliation is linear, the restriction of a polynomial of fixed maximal degree to a leaf is a polynomial of fixed maximal degree there, and thus we can apply the version of Friedrichs' Inequality from Theorem 2.38: Because the parameterisation for the normal extension is linear in the last κ variables for any fixed $x \in \omega$, polynomial degree is retained in these variables. Then for $R := P \circ \Psi - \vec{P} \circ \Psi$ we obtain the relation

$$\begin{aligned} & \int_{B_{c_1 h}[\xi]} (\partial_x^{\alpha_{\underline{k}}} R(x, z))^q dz dx \leq \int_{B_{c_3 h}[\Pi_\omega(\xi)]} (\partial_x^{\alpha_{\underline{k}}} R(x, z))^q dz dx \\ &= \int_{B_{c_3 h}^\omega[\xi] B_{c_3 h}^\kappa[0]} (\partial_x^{\alpha_{\underline{k}}} R(x, z))^q dz dx \leq c h^q \sum_{|\beta|=1} \|\partial_x^{\alpha_{\underline{k}}} \partial_z^\beta R\|_{L_q(B_{c_3 h}[\xi])}^q. \end{aligned} \quad (3.29.3)$$

Thereby, we have transformed the case $|\alpha| = |\alpha_{\underline{k}}|$ into the case $|\alpha + \beta| = |\alpha_{\underline{k}}| + 1$ with enhancement by some additional z -derivative ∂_z^β and maintain $|\alpha + \beta| < m$, $|\alpha + \beta| \leq n$. Since we have also gained h^q , we can handle this case right along with the other case and just consider α with $|\alpha_{\underline{k}}| > 0$ now: There holds $\partial^{\alpha_{\underline{k}}}(\vec{P} \circ \Psi) = \partial^{\alpha_{\underline{k}}}(\vec{F} \circ \Psi) = 0$, so we obtain

$$\partial_x^{\alpha_{\underline{k}}} \partial_y^{\alpha_{\underline{k}}} (P \circ \Psi - \vec{P} \circ \Psi) = \partial_x^{\alpha_{\underline{k}}} \partial_y^{\alpha_{\underline{k}}} (P \circ \Psi - \vec{F} \circ \Psi).$$

Hence, we have with the norm equivalences of Theorem 2.26 in particular, a suitable constant $c_4 \geq c_2$ such that $\Psi(B_{c_2 h}[\xi]) \subseteq B_{c_4 h}[\zeta]$ due to Lemma 3.25 and the approximation result from Lemma 3.28:

$$\begin{aligned} \|\partial^\alpha (P \circ \Psi - \vec{F} \circ \Psi)\|_{L_q(B_{c_3 h}[\xi])} &\leq c \sum_{|\beta| \leq |\alpha|} \|\partial^\beta (P - \vec{F})\|_{L_p(B_{c_4 h}[\zeta])} \\ &\leq c h^{n-|\alpha|} \|\vec{F}\|_{W_p^n(B_{mc_4 h}[\zeta])}. \end{aligned} \quad (3.29.4)$$

Possibly choosing h_0 smaller and \tilde{b} greater, we obtain thereby also for the second summand of (3.29.1) the relation

$$\begin{aligned} \|\partial^\alpha (P \circ \Psi - \vec{P} \circ \Psi)\|_{L_q(B_{c_1 h}[\xi])}^q &\leq \|\partial^\alpha (P \circ \Psi - \vec{F} \circ \Psi)\|_{L_q(B_{c_3 h}[\xi])}^q \\ &\leq c h^{q(n-|\alpha|)} \|\vec{F}\|_{W_p^n(B_{\tilde{b} h}[\zeta])}^q. \end{aligned} \quad (3.29.5)$$

Now we have to sum over all multi-indices α and obtain

$$\|f - p\|_{W_q^\mu(B_h[\zeta] \cap M)} \leq c h^{n-\mu-\kappa/q} \|\vec{F}\|_{W_q^n(B_{\tilde{b} h}[\zeta])}.$$

It remains to sum over all cell centers ζ . To this end, we have to choose \tilde{b} large enough to work out for each cell center ζ in at least one extended parameter space. This will be no problem if h_0 is small enough. We further have to take care that we choose some $b > 0$ large enough such that any $B_{\tilde{b} h}[\zeta]$ is contained in $U_{bh}(M)$ inde-

pendent of h . And we have to choose h_0 small enough to achieve that $U_{bh}(\mathcal{M})$ has the closest point property. Then because \tilde{b} was fixed over a fixed extended parameter space and the number of these is finite, we can choose \tilde{b} maximal among them to become independent of the extended parameter spaces. And because clearly any $z \in U_{bh}(\mathcal{M})$ can be in at most n_0 balls $B_{\tilde{b}h}[\zeta]$ for some fixed n_0 , we deduce

$$\sum_{\zeta \in \mathbb{Z}_{a,h}} \|f - p\|_{W_q^\mu(B_h[\zeta] \cap \mathcal{M})} \leq c h^{n-\mu-\kappa/q} \|\tilde{F}\|_{W_q^n(U_{bh}(\mathcal{M}))} \leq c h^{n-\mu} \|f\|_{W_q^n(\mathcal{M})}.$$

□

3.30 Remark: Again, if $\mathcal{M} \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ has a boundary, then the same holds at least for $S_h^N := R_M T_{\widehat{\mathcal{M}}} S_h E_N E_M^{\widehat{\mathcal{M}}}$, where $E_M^{\widehat{\mathcal{M}}}$ is the continuous extension operator that maps $W_q^n(\mathcal{M})$ to $W_q^n(\widehat{\mathcal{M}})$ for the $\widehat{\mathcal{M}} \in \mathbb{M}_{\text{cp}}^k(\mathbb{R}^d)$ such that $\mathcal{M} \Subset \widehat{\mathcal{M}}$.

3.3.4 Approximation in Fractional Orders and under fixed Interpolation Constraints

Both of the results for approximation by S_h^N we have presented so far allow for a generalisation to fractional Slobodeckij Hilbert spaces on ESMs. But in contrast to the Euclidean setting, we have to deal with the chart-wise definition of these spaces, and so the argumentation becomes more involved; the key ingredient is to determine two inverse atlases such that one is a restriction of the other. Such two inverse atlases are not hard to create in the case of an ESM *without* boundary we consider here: By compactness of the ESM, we can simply take sufficiently large compactly contained subsets of the parameter spaces of a given inverse atlas, restrict the parameterisations and still maintain an inverse atlas with all relevant properties. Then we can prove the following result:

3.31 Corollary

1. Let in the situation of Corollary 3.18 $0 < r \leq m$ and $0 \leq \varrho \leq \lfloor r - \kappa \rfloor$ be reals such that $\lfloor \varrho \rfloor < m - \kappa$. Then any $f \in H^r(\mathcal{M})$ satisfies the relation

$$\|f - S_h^N f\|_{H^\varrho(\mathcal{M})} \leq c h^{r-\varrho} \|f\|_{H^r(\mathcal{M})}.$$

This relation remains valid if one replaces extension operator E_N by any other foliation-based extension operator $E_{\mathbb{F}}$.

2. Let in the situation of Theorem 3.29 $0 < r \leq m$ and real $0 \leq \varrho \leq \lfloor r - 1 \rfloor$ be reals such that $\lfloor \varrho \rfloor < m - 1$. Then any $f \in H^r(\mathcal{M})$ satisfies the relation

$$\|f - S_h^N f\|_{H^\varrho(\mathcal{M})} \leq c h^{r-\varrho} \|f\|_{H^r(\mathcal{M})}.$$

This relation remains valid if one replaces extension operator E_N by any other extension operator E_V based on a linear foliation V .

Proof: With given inverse atlas $(\psi_i, \omega_i)_{i \in I} \in \mathbb{I}(\mathbb{M})$, we know by definition of $\mathbb{I}(\mathbb{M})$ that there is another inverse atlas $(\psi_i^*, \omega_i^*)_{i \in I}$ such that for any $i \in I$

$$\omega_i \subseteq \omega_i^* \quad \text{and} \quad \psi_i = (\psi_i^*)|_{\omega_i}.$$

Shrinking each ω_i just a little so that still $\omega_i \subseteq \omega_i^*$, we can further demand that actually $(\psi_i^*, \omega_i^*)_{i \in I} \in \mathbb{I}(\mathbb{M})$ as well. Then we will frequently apply the interpolation property from Proposition 2.30 for the operator $\text{Id} - S_h^N$ for different choices of the spaces and norms involved. Now we fix one (ψ, ω) and corresponding (ψ^*, ω^*) . We first have to deduce that in the situations of Corollary 3.18 or Theorem 3.29 for the respective choices of n, μ

$$\|(f - S_h^N f) \circ \psi\|_{H^\mu(\omega)} \leq c h^{n-\mu} \|f \circ \psi^*\|_{H^n(\omega^*)}. \quad (3.31.1)$$

To see this, we note that S_h^N is local in the following sense: For sufficiently small h we have that $\|(g - f) \circ \psi^*\|_{H^n(\omega^*)} = 0$ implies $\|(S_h^N(g - f)) \circ \psi\|_{H^\mu(\omega)} = 0$ for any $g \in H^n(\mathbb{M})$. In particular, this holds for $g = f^* := E_{\omega^*}^M f$ as obtained by the continuous manifold extension $E_{\omega^*}^M : H^n(\omega^*) \rightarrow H^n(\mathbb{M})$ of Theorem 2.36. And we have further that

$$\|f^*\|_{H^n(\mathbb{M})} \leq c \|f \circ \psi^*\|_{H^n(\omega^*)}.$$

This gives us directly (3.31.1). Then we apply the interpolation property. First, we choose suitable integers $n_1 = \lfloor \varrho \rfloor, n_2 = \lceil \varrho \rceil$ to which (3.31.1) applies if we set $\mu = \mu_i$. This is guaranteed if respectively either $n_2 \leq n - \kappa$ and $n_2 < m - \kappa$ (Corollary 3.18) or $n_2 \leq n - 1$ and $n_2 < m - 1$ (Theorem 3.29). Then we choose $0 < \theta < 1$ such that $\varrho = \theta n_1 + (1 - \theta)n_2$. We obtain for $m_1 = m_2 = n$ in the interpolation property for the operator $\text{Id} - S_h^N$ the relation

$$\begin{aligned} \|(f - S_h^N f) \circ \psi\|_{H^\varrho(\omega)} &\leq c h^{\theta(n-n_1)+(1-\theta)(n-n_1)} \|f \circ \psi^*\|_{H^n(\omega^*)} \\ &\leq c h^{n-\varrho} \|f \circ \psi^*\|_{H^n(\omega^*)}. \end{aligned} \quad (3.31.2)$$

The presence of the operation " $\circ \psi$ " therein does no harm, as we can always demand that an arbitrary $g \in H^n(\omega^*)$ has the form $g = \tilde{g} \circ \psi^*$ ⁽³⁾. Now we apply the interpolation property again for the choices $\varrho_1 = \varrho_2 = \varrho$ and $m_1 = \lfloor r \rfloor, m_2 = \lceil r \rceil$. By hypothesis, both choices satisfy the requirements for n , and so we have for $i = 1, 2$

⁽³⁾Therein, we can choose $\tilde{g} = R_{\omega^*} \Lambda_{(\psi^*)^{-1}} R_{\psi^*(\Omega^*)} E^* g$ for $E^* = E_{\mathbb{R}^d}^{\mathbb{R}^d} E_{\omega^*}^{\mathbb{R}^k}$, extended parameter space Ω^* corresponding to ω^* and $\Lambda_{(\psi^*)^{-1}}$ defined by $\Lambda_{(\psi^*)^{-1}} G = G \circ (\psi^*)^{-1}$. Then we have for an arbitrary $x \in \omega^*$ that $\tilde{g}(\psi^*(x)) = (E^* g)(x) = g(x)$ whenever g is smooth. As all operators that appeared were bounded, the general result then comes directly via density.

$$\|(f - S_h^N f) \circ \psi\|_{H^\varrho(\omega)} \leq c h^{m_i - \varrho} \|f \circ \psi^*\|_{H^{m_i}(\omega^*)},$$

and clearly $r = \theta m_1 + (1 - \theta)m_2$ for suitable $0 < \theta < 1$. We can do so by virtue of (3.31.2). Then we obtain the relation

$$\|(f - S_h^N f) \circ \psi\|_{H^\varrho(\omega)} \leq c h^{\theta(m_1 - \varrho) + (1 - \theta)(m_2 - \varrho)} \|f \circ \psi^*\|_{H^r(\omega^*)} = c h^{r - \varrho} \|f \circ \psi\|_{H^r(\omega^*)}.$$

To deduce the overall result, we have to sum over the two inverse atlases on both sides, which we can easily accomplish. And we have to see that, as one directly verifies, the two Sobolev norms on M subordinate to our two inverse atlases are equivalent. \square

3.32 Remark: Again, the case of an ESM with boundary can at least theoretically be deduced directly by extension operator $E_M^{\widehat{M}} : H^r(M) \rightarrow H^r(\widehat{M})$ for a compact submanifold \widehat{M} such that $M \Subset \widehat{M}$. Thereby, the same approximation orders as in the corollary are achievable at least theoretically.

Now we take the results on the boundedness of operators into account that we have proven in particular in Theorem 3.21. If we do that, we can also deduce results for approximation orders under fixed interpolation constraints. To be more precise, we obtain the following result on suitably constructed Ξ -interpolating quasi-projections that we shall apply in approximation of energy functional minima later:

3.33 Corollary *Let $E_M = E_M^{\mathbb{R}^d} : H^\varrho(M) \rightarrow H^{\varrho + \kappa/2}(\mathbb{R}^d)$ be the universal bounded extension operator and define the interpolating approximation operator as*

$$S_h^{\Xi, N} := T_M(S_h E_N + I_h^\Xi E_M - I_h^\Xi E_M T_M S_h E_N).$$

Then this operator retains the approximation orders of S_h^N according to Cor. 3.31 under the respective conditions, as long as in addition to the respective requirements it holds $k/2 < \varrho$ and $\varrho + \kappa/2 \leq m - 1$.

Proof: If we consider the approximation error, then for admissible ϱ by the triangle inequality

$$\|f - S_h^{\Xi, N} f\|_{H^\varrho(M)} \leq \|f - S_h^N f\|_{H^\varrho(M)} + \|T_M I_h^\Xi E_M (f - S_h^N f)\|_{H^\varrho(M)}.$$

So it suffices to prove continuity of $T_M I_h^\Xi E_M$, which is directly implied by its construction. \square

3.34 Remark: We use this last result only for deducing “achievable orders” — again it has only little practical value due to the presence of E_M . But in that respect, it is indeed very useful. And as usual, it generalises to the case of ESMs with

boundary by continuous (universal) extension from the ESM with boundary to the ESM without it is contained in by our assumptions.

3.3.5 Approximating Normal Derivatives

As an enhancement to the previous results, we will now be interested in the approximation power of the operator S_h^N when it comes to *normal* derivatives: These will soon turn out to tell us how large the deviation of tangent Euclidean derivatives to their intrinsic counterparts is, the *tangential derivatives* we introduce in chapter four. In the upcoming relations, we will always demand that the derivative D_N or gradient ∇_N is taken along the respective normal frame of the closest point if we are not on the ESM itself. And the index " N " indicates projection onto the normal space according to the specific, locally smooth map N that assigns an (orthonormal) normal frame to each element of the ESM.

The basic idea is now the same as in deriving the corresponding approximation results. We begin by stating them for integer orders and deduce the fractionals similar to Corollary 3.31 in the aftermath, which we complete by considering the case with interpolation constraints. We give proofs in correspondence to both Corollary 3.18 and Theorem 3.29, as the proof for the first will generalise also to other approximation methods and other orthogonal foliations easily, while the latter is more specific to splines and the normal foliation.

3.35 Corollary *Let in the situation of Cor. 3.18 holds in particular that $1 + \kappa \leq n$ and $1 + \kappa < m$ for $n \leq m \in \mathbb{N}$ defined there. Then the normal derivatives satisfy*

$$\|\nabla_N(S_h E_N f)\|_{2, L_2(M)} \leq c h^{n-1} \|f\|_{H^n(M)}.$$

Proof: In order to prove this result, we will essentially try to reduce things so far that dealing with $\|(\nabla_N S_h)\|_2$ reduces to a special case of the proof of Theorem 3.3. That proof had started from a pair of parameterisation and parameter space (ψ, ω) , according to the inverse atlas to obtain (3.3.1). To obtain a similar relation, we have to look at our usual map $N = (v^1, \dots, v^k)$ giving us a normal frame on the image of ω that is smooth and C -bounded on ω , of which we know it exists. We decompose then $\|(\nabla_N S_h)\|_2$ as follows in a finite sum of normal directional derivatives: It holds in any $\psi(x)$ for $x \in \omega$ that

$$\|\nabla_N S_h\|_2^2 = \sum_{\ell=1}^K |D_{v^\ell} S_h|^2 \leq c \left(\sum_{\ell=1}^K |D_{v^\ell} S_h| \right)^2 = c \|\nabla_N S_h\|_1^2,$$

and consequently we have with the triangle inequality in the last step

$$\|(\nabla_N S_h)\|_2\|_{L_2(\Psi(\omega))} \leq c \|(\nabla_N S_h) \circ \Psi\|_1\|_{L_2(\omega)} \leq c \sum_{i=1}^K \|(\mathcal{D}_{\nu^i} S_h) \circ \Psi\|_{L_2(\omega)}. \quad (3.35.1)$$

Then we choose an arbitrary $\mathcal{D}_{\nu} = \mathcal{D}_{\nu^j}$ and define Ω_{ah} as in the proof of Theorem 3.3. We can thus obtain as in (3.3.1) that because $\mathcal{D}_{\nu} \vec{F} = 0$ it holds

$$\begin{aligned} \|(\mathcal{D}_{\nu} S_h) \circ \Psi\|_{L_2(\omega)} &\leq c h^{-\frac{\kappa}{2}} \|E_N(\mathcal{D}_{\nu} S_h) \circ \Psi\|_{L_2(\Omega_{ah})} \\ &= c h^{-\frac{\kappa}{2}} \|E_N(\mathcal{D}_{\nu} S_h) \circ \Psi - (\mathcal{D}_{\nu} \vec{F}) \circ \Psi\|_{L_2(\Omega_{ah})} \\ &\leq c h^{-\frac{\kappa}{2}} \|(\mathcal{D}_{\nu} S_h) \circ \Psi - (\mathcal{D}_{\nu} \vec{F}) \circ \Psi\|_{L_2(\Omega_{ah})} \\ &\quad + c h^{-\frac{\kappa}{2}} \|(\mathcal{D}_{\nu} S_h) \circ \Psi - E_N(\mathcal{D}_{\nu} S_h) \circ \Psi\|_{L_2(\Omega_{ah})}. \end{aligned}$$

Now we have to notice that on Ω_{ah} we have that by definition of N and its component column $\nu = \nu^j$ it holds $(\mathcal{D}_{\nu} S_h) \circ \Psi = \partial_j(S_h \circ \Psi)$ for some standard coordinate direction j . This can be deduced directly from the definition of Ψ . The first summand can then be bounded by using the evident relation $|\mathcal{D}_{\nu}(S_h - \vec{F})| \leq \|\nabla(S_h - \vec{F})\|_2$ in the form

$$\begin{aligned} \|(\mathcal{D}_{\nu}(S_h - \vec{F})) \circ \Psi\|_{L_2(\Omega_{ah})} &\leq \|(S_h - \vec{F}) \circ \Psi\|_{H^1(\Omega_{ah})} \\ &\leq c \|S_h - \vec{F}\|_{H^1(U_{ah})} \leq h^{n-1} \|\vec{F}\|_{H^n(U_{bh})}. \end{aligned}$$

For the second summand, we are by definition in the case of $|\alpha^{\kappa}| = 0$ of the respective proof, and thus proceed similarly via Friedrichs' inequality to obtain for $R_h := (\mathcal{D}_{\nu} S_h) \circ \Psi - (E_N(\mathcal{D}_{\nu} S_h)) \circ \Psi$ the relation

$$\|R_h\|_{L_2(\Omega_{ah})}^p \leq c \sum_{\ell=1}^K h^{p \cdot \ell} \sum_{|\beta|=\ell} \|\partial_z^{\beta} R_h\|_{L_p(\Omega_{ah})}^p. \quad (3.35.2)$$

Now we notice that it holds $(E_N(\mathcal{D}_{\nu} S_h))(\Psi(x, z)) = (E_N(\mathcal{D}_{\nu} S_h))(\Psi(x, 0))$, whereby in particular $\partial_z^{\beta}((E_N(\mathcal{D}_{\nu} S_h)) \circ \Psi) = 0 = \partial_z^{\beta} \partial_j(\vec{F} \circ \Psi)$. Consequently we can deduce by virtue of Friedrichs' inequality that it holds

$$\begin{aligned} \|R_h\|_{L_2(\Omega_{ah})}^p &\leq c \sum_{\ell=1}^K h^{p \cdot \ell} \sum_{|\beta|=\ell} \|\partial_z^{\beta} \partial_j(S_h \circ \Psi - \vec{F} \circ \Psi)\|_{L_p(\Omega_{ah})}^p \\ &\leq c \sum_{\ell=1}^K h^{p \cdot \ell} \sum_{|\eta|=\ell+1} \|\partial_z^{\eta}(S_h \circ \Psi - \vec{F} \circ \Psi)\|_{L_p(\Omega_{ah})}^p. \end{aligned}$$

Because we have required that $\kappa + 1 < m$ and $\kappa + 1 \leq n$, we can proceed as before in (3.3.4) and obtain via the usual norm equivalences for any of the shifted multi-indices η in the last sum that

$$\|\partial_z^{\eta} R_h\|_{L_2(\Omega_{ah})}^p \leq \|\partial_z^{\eta}(S_h \circ \Psi - \vec{F} \circ \Psi)\|_{L_2(\Omega_{ah})} \leq c h^{(n-\mu-|\eta|)p+\kappa} \|f\|_{H^n(\mathcal{M})}^2,$$

whereby the desired result is obtained by insertion and summation. Note in particular that $\nabla_N S_h$ is given by a finite linear combination of normal directional derivatives on each pair (ψ, ω) according to the inverse atlas and that the overall result is invariant under orthogonal transformation within the normal space. \square

3.36 Corollary *In the situation of Theorem 3.29 it holds as long as in particular $2 \leq n$ and $2 < m$ that the normal derivatives satisfy*

$$\|\nabla_N(S_h E_N f)\|_{2, L_2(M)} \leq c h^{n-1} \|f\|_{H^n(M)}.$$

Proof: Again, the proof is very similar to that of 3.29: We have to reuse the decomposition of (3.35.1) and replace as in the last proof s_h in the proof of 3.35 by $(D_\nu S_h)|_M$ and consequently p in the proof of 3.35 by $D_\nu P$ for an arbitrary $D_\nu = D_{\nu^i}$ in the respective relations. Then we obtain similar to (3.29.1) that

$$\begin{aligned} \int_{\omega \cap B_{c_1 h}[\xi]} ((D_\nu P) \circ \Psi)^2 &\leq c h^{-\kappa} \int_{B_{c_1 h}[\xi]} ((D_\nu \vec{F}) \circ \Psi - (D_\nu P) \circ \Psi)^2 \\ &\quad + c h^{-\kappa} \int_{B_{c_1 h}[\xi]} ((D_\nu P) \circ \Psi - (E_N(D_\nu P)) \circ \Psi)^2. \end{aligned}$$

For the first summand, we conclude similar to (3.29.2) that

$$\int_{B_{c_1 h}[\xi]} ((D_\nu \vec{F}) \circ \Psi - (D_\nu P) \circ \Psi)^2 \leq c h^{2(n-1)} \|\vec{F}\|_{H^n(B_{mc_2 h}[\xi])}^q.$$

Therein, we use as in the previous proof that for an arbitrary G it holds $(D_{\nu^j} G) \circ \Psi = \partial_j(G \circ \Psi)$. For the second summand, we can also proceed as before and apply Friedrichs' Inequality for leafwise finite dimensional polynomials: The directional derivative along a normal is again a polynomial. So we obtain also in this case similar to (3.29.3) that for $R_h := ((D_\nu P) \circ \Psi - (E_N(D_\nu P)) \circ \Psi)$

$$\int_{B_{c_1 h}[\xi]} (R_h)^2 \leq c h^2 \sum_{|\beta|=1} \|\partial_z^\beta(R_h)\|_{L_2(B_{c_3 h}[\xi])}^2.$$

Now we repeat the observations made in the proof of Corollary 3.35 after deducing (3.35.2). Thereby we obtain again for j as implied by $\nu = \nu^j$

$$\begin{aligned} \sum_{|\beta|=1} \|\partial_z^\beta(R_h)\|_{L_2(B_{c_3 h}[\xi])}^2 &= \sum_{|\beta|=1} \|\partial_z^\beta(\partial_j(P \circ \Psi))\|_{L_2(B_{c_3 h}[\xi])}^2 \\ &\leq \sum_{|\beta|=2} \|\partial_z^\beta(\vec{F} \circ \Psi - P \circ \Psi)\|_{L_2(B_{c_3 h}[\xi])}^2. \end{aligned}$$

Once again, this gives us as in (3.29.4) that

$$\int_{B_{c_1 h}[\xi]} ((D_\nu P) \circ \Psi - (E_N(D_\nu P)) \circ \Psi)^2 \leq c h^{2n-2} \|\vec{F}\|_{H^n(B_{mc_4 h}[\zeta])}^2.$$

Now we can proceed precisely as in the proof of 3.29. □

3.37 Corollary *In the situation of Cor. 3.31 it holds, as long as in particular $\varrho = 1$ is a valid choice, that normal derivatives satisfy the relation*

$$\|\nabla_N(S_h E_N f)\|_{2, L_2(M)} \leq c h^{r-1} \|f\|_{H^r(M)}.$$

Proof: As in the proof of Cor. 3.31 we hope to apply the interpolation property. Thus we choose again the two inverse atlases from the proof of that corollary. For parameterisation ψ^* and parameter space ω^* according to the inverse atlas we can choose N^* smooth on ω^* and restrict ourselves once again to arbitrary column $\nu = \nu^j$. Then the linear map $f \mapsto T_M D_\nu(S_h^N f)$ is by virtue of the last two corollaries bounded from $H^{m_i}(\omega^*)$ to $L_2(\omega)$ and it holds

$$\|(D_\nu(S_h^N f)) \circ \psi\|_{L_2(\omega)} \leq c h^{m_i-1} \|f \circ \psi^*\|_{H^{m_i}(\omega^*)},$$

for any m_i , $i = 1, 2$ that are valid choices for n , in particular for $m_1 = \lfloor r \rfloor$ and $m_2 = \lceil r \rceil$. With a suitable choice for $0 < \theta < 1$ such that $r = \theta m_1 + (1 - \theta)m_2$ we conclude then by the interpolation property

$$\|(D_\nu(S_h^N f)) \circ \psi\|_{L_2(\omega)} \leq c h^{r-1} \|f \circ \psi^*\|_{H^r(\omega^*)}.$$

Thereby we can deduce as before that

$$\|(\nabla_N(S_h^N f)) \circ \psi\|_{2, L_2(\omega)} \leq c h^{r-1} \|f \circ \psi^*\|_{H^r(\omega^*)}.$$

Again, finite summation yields the desired result. □

To deduce a result for the case with interpolation constraints requires another auxiliary result stated in the following lemma:

3.38 Lemma *Let $G \in H^r(U(M))$ for $r \geq 2$. Then for any $\varepsilon > 0$ with $\kappa/2 + \varepsilon \leq r - 1$*

$$\|\nabla_N G\|_{2, L_2(M)} \leq c \|G\|_{H^{1+\kappa/2+\varepsilon}(U(M))}.$$

Proof: We choose an inverse atlas $(\psi_i, \omega_i)_{i \in I}$ for M and corresponding extended

inverse atlas $(\Psi_i, \Omega_i)_{i \in I}$ for $U(M)$. Then we select again arbitrary but corresponding $(\psi, \omega), (\Psi, \Omega)$ according to these, omitting the index i from now on for this specific choice. By construction of Ψ and Ω , we can demand that on $\Psi(\Omega)$ the map $x \mapsto N(\Pi_M(x))$ is well-defined, smooth and C -bounded. We call by ν^1, \dots, ν^k the columns of orthonormal normal frame N again and choose as before an arbitrary $\nu = \nu^j$. First we demand G to be smooth and state that it holds for the directional derivative $D_\nu G$ of G along ν that $|D_\nu G|^2 \leq c \|\nabla G\|_2^2$ both on $\psi(\omega)$ and on $\Psi(\Omega)$. Moreover, we even have for any $\sigma \geq 0$ such that $G \in H^{1+\sigma}(U(M))$ also

$$\|(D_\nu G)\|_{H^\sigma(\Psi(\Omega))} \leq c \|G\|_{H^{1+\sigma}(\Psi(\Omega))} \leq c \|G\|_{H^{1+\sigma}(U(M))}.$$

This is obvious for $\sigma = 0$. For $\sigma = n \in \mathbb{N}$ we can obtain this by the product rule and the fact that N can be presumed to be C -bounded on $\Psi(\Omega)$. Induction and the triangle inequality give then the required result. Consequently, we can also deduce (via density) that the map $G \mapsto D_\nu G$ is in fact a bounded linear map from $H^m(\Psi(\Omega))$ to $H^{m-1}(\Psi(\Omega))$ for all $m \in \mathbb{N}$.

Now we apply the interpolation property. So let ϱ be fractional and choose $0 < \theta < 1$ such that $\varrho = \theta[\varrho] + (1 - \theta)[\varrho]$. Then an easy calculation shows that

$$\varrho - 1 = \theta[\varrho] + (1 - \theta)[\varrho] - 1 = \theta[\varrho - 1] + (1 - \theta)[\varrho - 1].$$

Thus by the interpolation property from Proposition 2.30 the map is also bounded from $H^\varrho(\Psi(\Omega))$ to $H^{\varrho-1}(\Psi(\Omega))$. This gives us the fractional case. To deduce the claimed relation, we have first to see that

$$\|\nabla_N G\|_{L_2(\psi(\omega))}^2 = \sum_{\ell=1}^K \int_{\psi(\omega)} |D_{\nu^\ell(x)} G|^2 dx.$$

Then obviously $\|(D_\nu G)\|_{L_2(\psi(\omega))} \leq \|(D_\nu G)\|_{H^\varepsilon(\psi(\omega))}$ for any $\varepsilon > 0$. By the chart trace theorem, so Theorem 2.33, it holds in particular that

$$\|(D_\nu G)\|_{H^\varepsilon(\psi(\omega))} \leq c \|(D_\nu G)\|_{H^{\varepsilon+K/2}(\Psi(\Omega))}$$

and by our previous findings this is bounded by $c \|G\|_{H^{1+\varepsilon+K/2}(U(M))}$. To deduce the ultimate relation, we just have to sum over the finite inverse atlas. \square

3.39 Corollary *Let in the situation of the last corollaries $\Xi \subseteq M$ be a finite set of points. Then it holds with the operator $S_h^{\Xi, N}$ instead of S_h^N and with*

$$S_h^{\Xi, N, U} := S_h E_N + I_h^\Xi E_M - I_h^\Xi E_M T_M S_h E_N$$

its result before application of T_M that for any small $\varepsilon > 0$

$$\|\nabla_N (S_h^{\varepsilon, N, U} f)\|_2 \Big|_{L_2(\mathcal{M})} \leq c h^{r-\max(1, k/2)-\varepsilon} \|f\|_{H^r(\mathcal{M})}.$$

Proof: We start with the triangle inequality to obtain

$$\|\nabla_N (S_h^{\varepsilon, N, U} f)\|_2 \Big|_{L_2(\mathcal{M})} \leq \|\nabla_N (S_h E_N f)\|_2 \Big|_{L_2(\mathcal{M})} + \|\nabla_N ((I_h^{\varepsilon} E_M - I_h^{\varepsilon} E_M T_M S_h E_N) f)\|_2 \Big|_{L_2(\mathcal{M})}.$$

The first summand is then bounded by the respective property of S_h^N . For the second summand, we apply Lemma 3.38 and obtain for some fixed $U(\mathcal{M})$ that

$$\|\nabla_N ((I_h^{\varepsilon} E_M - I_h^{\varepsilon} E_M T_M S_h E_N) f)\|_2 \Big|_{L_2(\mathcal{M})} \leq c \|(I_h^{\varepsilon} E_M - I_h^{\varepsilon} E_M T_M S_h E_N) f\|_{H^{1+\kappa/2+\varepsilon}(U(\mathcal{M}))}.$$

We use the continuity of I_h^{ε} and conclude with $\kappa_{\varepsilon} = \kappa/2 + \varepsilon$

$$\begin{aligned} & \|(I_h^{\varepsilon} E_M - I_h^{\varepsilon} E_M T_M S_h E_N) f\|_{H^{1+\kappa_{\varepsilon}}(U(\mathcal{M}))} \\ & \leq \|(I_h^{\varepsilon} E_M - I_h^{\varepsilon} E_M T_M S_h E_N) f\|_{H^{\max(1, k/2)+\kappa_{\varepsilon}}(U(\mathcal{M}))} \\ & \leq \|(E_M - E_M T_M S_h E_N) f\|_{H^{\max(1, k/2)+\kappa_{\varepsilon}}(U(\mathcal{M}))} \\ & \leq \|(E_M - E_M T_M S_h E_N) f\|_{H^{\max(1, k/2)+\kappa_{\varepsilon}}(\mathbb{R}^d)} \\ & \leq \|(\text{Id} - T_M S_h E_N) f\|_{H^{\max(1, k/2)+\varepsilon}(\mathcal{M})} \\ & \leq c h^{r-\max(1, k/2)-\varepsilon} \|f\|_{H^r(\mathcal{M})}. \end{aligned}$$

□

3.40 Remark: Like for the previous statements on approximation by constant extension and restriction, the case of an ESM with boundary can at least theoretically be deduced directly by extension operator $E_M : H^r(\mathcal{M}) \rightarrow H^r(\widehat{\mathcal{M}})$ for a compact submanifold $\widehat{\mathcal{M}} \in \mathbb{M}_{\text{cp}}^k(\mathbb{R}^d)$ such that $\mathcal{M} \Subset \widehat{\mathcal{M}}$. Thereby, the same approximation orders are achievable at least theoretically.

3.41 Remark: It is also important to have approximation results just for the approximation of the normal derivatives in the ambient space: They help us to determine that an additional stabilisation penalty on the approximation in the ambient space which will occur later does not affect the approximation order. In case we have no interpolation constraints, it is directly clear that for any tubular neighbourhood $U_{ah}(\mathcal{M})$ that is sufficiently narrow we have the relation

$$\begin{aligned} \|\nabla_N (S_h E_N f)\|_2 \Big|_{L_2(U_{ah}(\mathcal{M}))} & \leq \|(S_h \vec{F} - \vec{F})\|_{H^1(U_{ah}(\mathcal{M}))} \\ & \leq \|(S_h \vec{F} - \vec{F})\|_{H^1(U_{ah_0}(\mathcal{M}))} \leq c h^{r-1} \|f\|_{H^r(\mathcal{M})}. \end{aligned}$$

The last inequality therein comes by application of Appendix Theorem 9.17 that gives the relation $\|\vec{F}\|_{H^r(U(M))} \leq c \|f\|_{H^r(M)}$. In fact, we could even expect to have higher orders, but that will play no significant role for us. In the case with a finite set of constraints, we have the relation

$$\|\nabla_N(S_h^{\varepsilon,N,U} f)\|_{L_2(U_{ah}(M))} \leq c h^{r-\max(1,k/2)} \|f\|_{H^r(M)}.$$

This is obtained via the intermediate steps

$$\begin{aligned} \|\nabla_N(S_h^{\varepsilon,N,U} f)\|_{L_2(U_{ah})} &= \|\nabla_N(E_N f - S_h^{\varepsilon,N,U} f)\|_{L_2(U_{ah})} \leq c \|(E_N f - S_h^{\varepsilon,N,U} f)\|_{H^1(U_{ah})} \\ &\leq c \|(S_h \vec{F} - \vec{F})\|_{H^1(U_{ah})} + c \|(I_h^{\varepsilon} E_M - I_h^{\varepsilon} E_M T_M S_h E_N) f\|_{H^1(U_{ah})} \\ &\leq c \|(S_h \vec{F} - \vec{F})\|_{H^1(U_{ah_0})} + c \|(I_h^{\varepsilon} E_M - I_h^{\varepsilon} E_M T_M S_h E_N) f\|_{H^1(U_{ah_0})} \\ &\leq c \|(S_h \vec{F} - \vec{F})\|_{H^1(U_{ah_0})} + c \|I_h^{\varepsilon} E_M (\text{Id} - T_M S_h E_N) f\|_{H^{\max(1,d/2)}(U_{ah_0})} \\ &\leq c \|(S_h \vec{F} - \vec{F})\|_{H^1(U_{ah_0})} + c \|(\text{Id} - S_h^N) f\|_{H^{\max(1,d/2)-\kappa/2}(M)} \\ &\leq c (h^{r-1} + h^{r-\max(1-\kappa/2,k/2)}) \|f\|_{H^r(M)} \leq c h^{r-\max(1,k/2)} \|f\|_{H^r(M)}. \end{aligned}$$

3.3.6 Practical Examples

The approximation operator S_h^N gives rise to a concept recently developed ([74, 75, 76, 82]) under the term *Ambient B-Spline Method* or more generally *Ambient Approximation Method* for codimension one, and by our theory the approach generalises naturally to higher codimensions. The process of the method is briefly described as follows:

3.42 Algorithm — Ambient B-Spline Method —

1. For h small, determine all the cells $C_h(M)$ active on M .
2. Compute⁽⁴⁾ the approximation of $F = f \circ \Pi_M^{(5)}$ for $C_h(M)$.
3. Store the coefficients just for the basis functions active on M to determine a solution S_M .
4. Evaluate S_M in points on M as necessary.

Initially, this algorithm was investigated for codimension $\kappa = 1$ alone ([74],[82]), and convergence rates were also investigated just for codimension one: [82] provides practical results that verify the theoretical orders for several types of surfaces in \mathbb{R}^3 . So in our examples we put our focus exemplarily on $\kappa = 2$ and thus on a

⁽⁴⁾This may require additional cells as required by the applied quasi-projection method. Usually one will need at least all cells active on some $U_{\delta h}(M)$ for fixed $\delta > 0$.

⁽⁵⁾Another suitable projection $\Pi_{\mathbb{F}}$ based on foliation \mathbb{F} is conceivable as well.

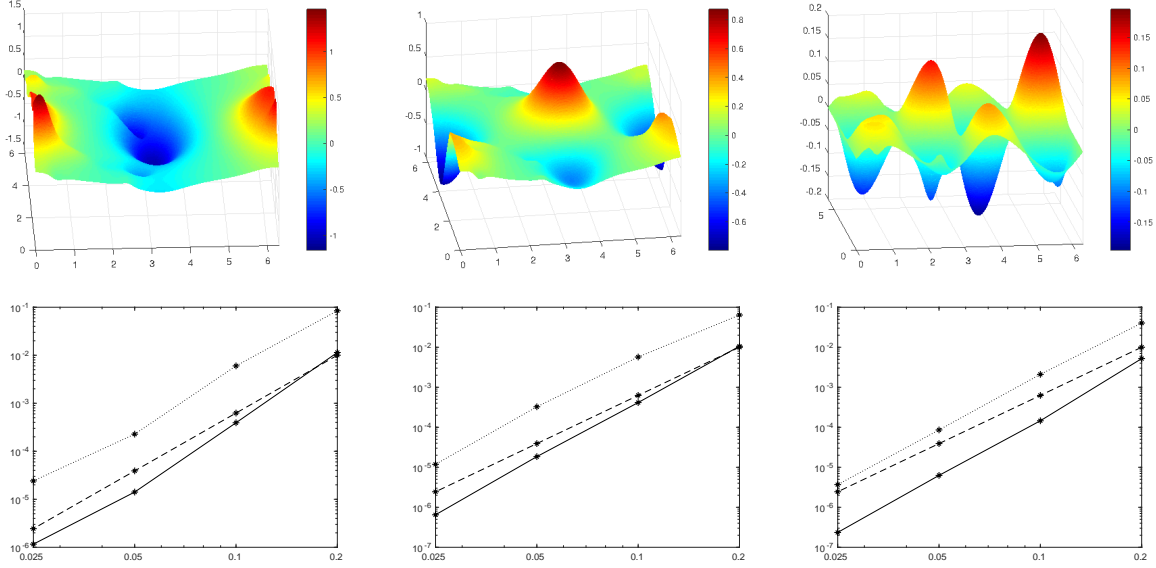


Figure 3.1: Upper row: Plots of the functions f_1 (left), f_2 (mid), f_3 (right). Lower row: Corresponding experimental rates of convergence for quadcubic splines: — root mean square error for 160^2 equally spaced gridded points, --- reference h^4 , maximal error.

surface embedded in \mathbb{R}^4 that is not embedded in \mathbb{R}^3 . To be more precise, we give examples in the case of the so called *Clifford torus* $\mathbb{T}_{\text{clf}} \subseteq \mathbb{R}^4$ — a surface which is not embedded into \mathbb{R}^3 and given as

$$\mathbb{T}_{\text{clf}} = \left(\frac{1}{\sqrt{2}} \mathbb{S}^1 \right) \times \left(\frac{1}{\sqrt{2}} \mathbb{S}^1 \right),$$

whereby one sees that it has a globally defined normal frame and can be parameterised by parameterisations of the circles. Consequently, it is isometrically isomorphic to $[0, \pi\sqrt{2}] \times [0, \pi\sqrt{2}]$ if one identifies opposite edges, and thus we can visualise functions on the Clifford torus in the plane — which we did on $[0, 2\pi] \times [0, 2\pi]$ for technical reasons, as implied by the standard parameterisation of the circle.

We present convergence behaviour for three functions f_1, f_2, f_3 on \mathbb{T}_{clf} that are defined as restrictions of the \mathbb{R}^4 functions F_1, F_2, F_3 given as

$$\begin{aligned} F_1(w, x, y, z) &:= e^{wz} w \left(\frac{3}{4} e^{-\frac{(9x+w-2)^2 + (9y+z-2)^2}{4}} + \frac{3}{4} e^{-\frac{(9x+1)^2}{49} - \frac{9y+1}{10}} \right) \\ &\quad + e^{wz} w \left(\frac{1}{2} e^{-\frac{(9x+w-7)^2 + (9y+z-3)^2}{4}} - \frac{1}{5} e^{-(9x+w-4)^2 - (9y+z-7)^2} \right) \\ F_2(w, x, y, z) &:= e^{wz} w(y+z) \left(\frac{3}{4} e^{-\frac{(9x+6w-2)^2 + (9y+6z-2)^2}{4}} + \frac{3}{4} e^{-(9x+1)^2/49 - (9y+1)/10} \right) \\ &\quad + e^{wz} w(y+z) \left(\frac{1}{2} e^{-\frac{(9x+w-7)^2 + (9y+z-3)^2}{4}} - \frac{1}{5} e^{-(9x+w-4)^2 - (9y+z-7)^2} \right) \\ F_3(w, x, y, z) &:= \frac{3}{4} (y+z) \sin(wz) \cos(w) e^{-\frac{(9x+6w-2)^2 + (9y+6z-2)^2}{4}} \end{aligned}$$

$$\begin{aligned}
& + \frac{3}{4}(y+z) \sin(wz) \cos(w) \frac{3}{4} e^{-(9x+1)^2/49-(9y+1)/10} \\
& + \frac{1}{2}(y+z) \sin(wz) \cos(w) e^{-\frac{(9x+w-7)^2+(9y+z-3)^2}{4}} \\
& - \frac{1}{5}(y+z) \sin(wz) \cos(w) e^{-(9x+w-4)^2-(9y+z-7)^2}.
\end{aligned}$$

Our approximations are computed by cubic TP-splines on \mathbb{R}^4 , so "quadcubics", with cell widths $h = 0.2, 0.1, 0.05, 0.025$ and provide precisely our estimations of h^4 convergence.

3.43 Remark: In our tests, we use the second variant for quasi-projection, the one performed in parallel on all cells in the support, as proposed in 3.14. We found that it has no significant negative impact on the expected rate of convergence if just the average over all cells active on a small tubular neighbourhood of \mathbf{M} was taken, and not necessarily all cells in the supports of all B-splines active on that neighbourhood. Thereby, the computational cost can be reduced by a significant constant factor.

We tested also an approximation based on extension along a linear foliation that is *not* the normal foliation: The foliation presented in Example 2.20. This has the significant advantage that we can circumvene the problem that the tubular neighbourhood may be very small if we require the closest point property. We illustrate this with the "unit balls" of the norms $\|\cdot\|_{64}, \|\cdot\|_{24}, \|\cdot\|_6$, so the zero surfaces of the maps

$$\begin{aligned}
(x, y, z) &\mapsto x^{64} + y^{64} + z^{64} - 1, \\
(x, y, z) &\mapsto x^{24} + y^{24} + z^{24} - 1, \\
(x, y, z) &\mapsto x^6 + y^6 + z^6 - 1.
\end{aligned}$$

In particular the first two would demand a neighbourhood so narrow that we can hardly afford it in practice, while the foliation \mathbb{V}_S along the normalised position vectors and the corresponding extension E_V are effectively well defined in all of $\mathbb{R}^d \setminus \{0\}$.

We tested with the restrictions of the functions

$$\begin{aligned}
F_4(x, y, z) &:= \frac{1}{4} \left(e^{-\frac{(9x-2)^2+(9y-2)^2}{4}} + e^{-\frac{(9x+1)^2}{49} - \frac{9y+1}{10}} \right) \\
&\quad + \frac{1}{4} \left(3e^{-\frac{(9x-7)^2+(9y-3)^2}{4}} - e^{-(9x-4)^2-(9y-7)^2} \right), \\
F_5(x, y, z) &:= \log(x^1 + y^3 + z^5 + 7)^{1/4}.
\end{aligned}$$

The functions on the respective surfaces and the corresponding convergence plots are presented in Fig. 3.2. We can see that the expected convergence is present.

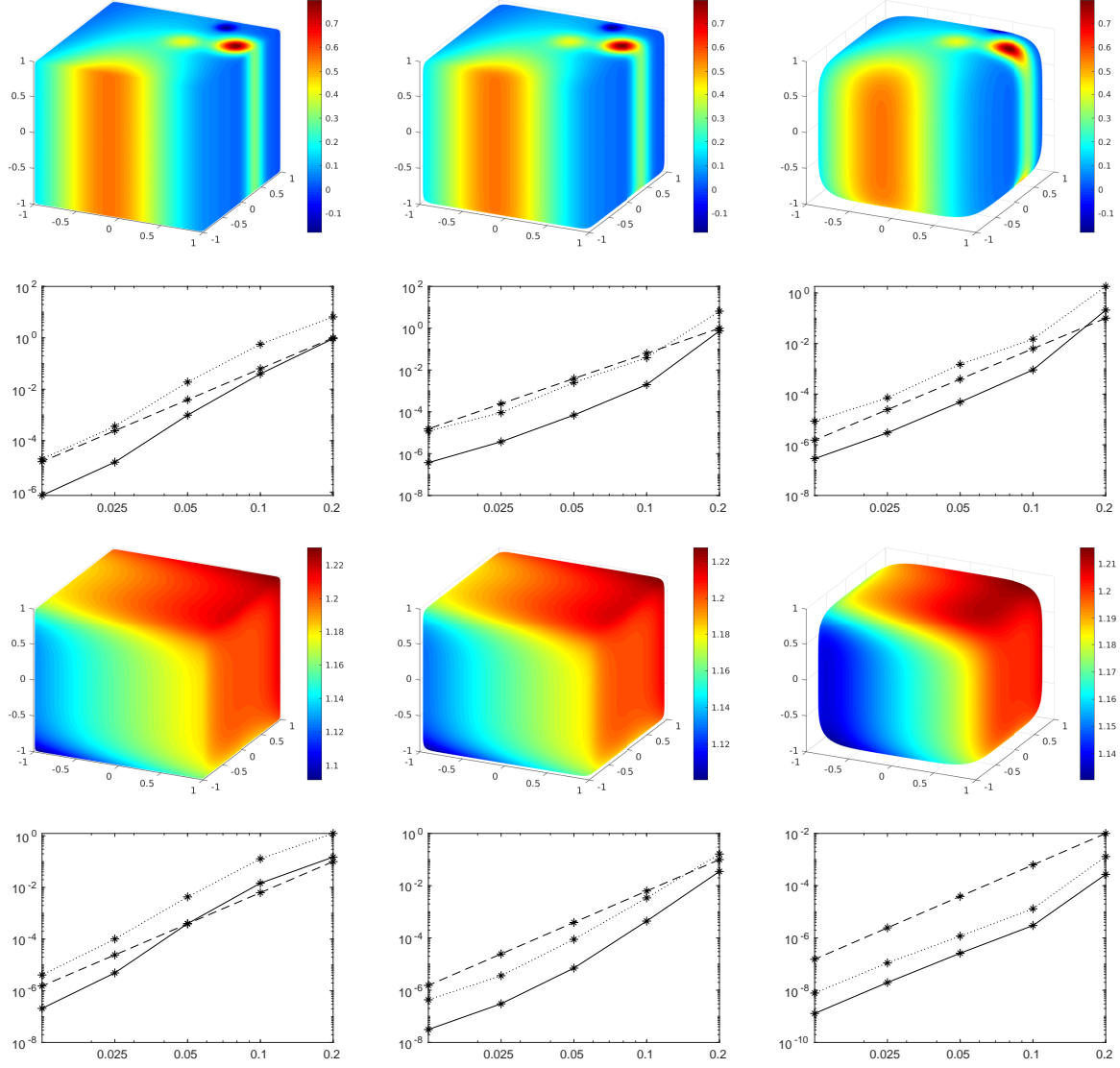


Figure 3.2: Upper row: Plots of the restrictions of function F_4 (first row) and F_5 (third row) to the respective surfaces functions. Second and fourth row: Corresponding experimental rates of convergence for tricubic splines: — root mean square error for $\approx 100'000$ roughly uniformly spaced points, --- reference h^4 , maximal eError.

And we can also see that the approximation results are satisfactory for choices of h that are far greater than any choice of h that would be possible for normal foliation \mathbb{F}_N and normal extension E_N .

And finally, we also tested the approximation behaviour for functions of limited regularity. To accomplish this, we relied on an idea proposed and applied e.g. in [49]: The authors used suitable interpolants by Matern-kernels to data sites on M to accomplish functions that are in $H^{\beta-\varepsilon}(M)$ for arbitrary choice of $\beta > k/2$ and any $0 < \varepsilon < \frac{1}{2}$; We did the same, for choices of $\beta \in \{1.5, 2.0, 2.5, 3.0\}$. Note in particular that the case $\beta = 1.5$ can only be handled by our fractional corollary to Theorem 3.29, but not by the same corollary to the spline version of Theorem 3.3.

We performed tests for functions on \mathbb{S}^2 and on the Clifford torus; these simple surfaces were chosen because we wanted to avoid effects of the geometry with large h . The functions employed in the tests are obtained as Matern kernel interpolants for

$$e_1 \mapsto 1.1, e_2 \mapsto 1.2, e_3 \mapsto 1.3, -e_1 \mapsto 1.4, -e_2 \mapsto 1.5, -e_3 \mapsto 1.6$$

in case of \mathbb{S}^2 , and for the Clifford torus as interpolants that satisfy

$$\begin{aligned} \frac{e_1 + e_3}{\sqrt{2}} &\mapsto 1.1, \frac{-e_1 + e_3}{\sqrt{2}} \mapsto 1.2, \frac{-e_2 + e_4}{\sqrt{2}} \mapsto 1.4, \frac{-e_2 - e_4}{\sqrt{2}} \mapsto 1.8, \\ \frac{-e_1 - e_3}{\sqrt{2}} &\mapsto 1.3, \frac{e_1 - e_3}{\sqrt{2}} \mapsto 1.5, \frac{e_2 + e_4}{\sqrt{2}} \mapsto 1.7, \frac{e_2 - e_4}{\sqrt{2}} \mapsto 1.9. \end{aligned}$$

Again, we find the expected rates of convergence verified in Fig. 3.3.

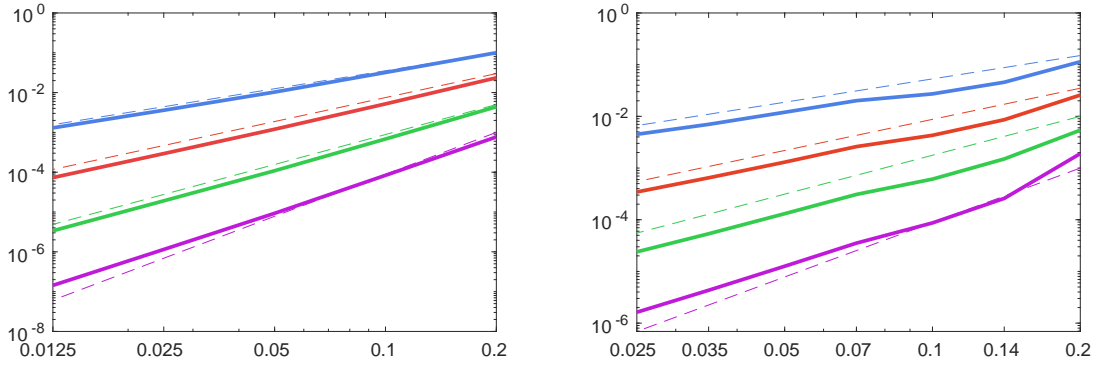


Figure 3.3: Convergence plots for approximation of functions of limited regularity on \mathbb{S}^2 (left) and the Clifford torus (right). References are depicted dashed, practical results solid and thicker: $f \in H^{\beta-\varepsilon}(\mathcal{M})$ and reference $\approx h^\beta$ for $\beta = 1.5$ (blue), $\beta = 2.0$ (red), $\beta = 2.5$ (green), $\beta = 3.0$ (purple).

Chapter 4

Tangential Calculus, Function Spaces and Functionals

Handling differential calculus in an ESM with an inverse atlas is in theory always possible, but it has significant drawbacks: For example, derivatives depend on the chosen parameterisations and have to be made invariant with quite some effort. Furthermore, whenever it comes to practical applications, the blending of chartwise solutions can pose significant difficulties, and it will directly affect the solution and its properties. Therefore, a purely intrinsic differential calculus is highly desirable. It should, of course, lead to equivalent norms etc. when talking about Sobolev spaces, and it should reduce to the standard calculus if the manifold considered is some open set in \mathbb{R}^k . To introduce such calculus and to investigate its properties is the prime objective of this chapter.

Specifically, we are first going to present an intrinsic *tangential* calculus for C^2 -functions. Next, we will use this to give an intrinsic characterisation of second order Hilbert space norms on ESMs based on that tangential calculus. After this, we will investigate when a finite set of points $\Xi \subseteq M$ ensures the only function $f : M \rightarrow \mathbb{R}$ with $f(\xi) = 0$ for all $\xi \in \Xi$ whose tangential counterpart of the Hessian vanishes identically will vanish identically itself on M . Thereby, we transfer the question of polynomial *unisolvency* to ESMs. In particular, we will find that for a wide range of ESMs only constant functions have identically vanishing Hessians. Afterwards, we will employ these results in problems of extrapolation and energy minimisation for a finite set of points, and use the general framework we introduce thereby to handle also more general energy minimisation problems and functionals, and the solution of certain intrinsic partial differential equations.

Finally, we will introduce the concept of *equivalently E_N -extrinsic functionals* or in short *E_N -extrinsic functionals* as functionals where tangential and Euclidean calculus are somehow mutually exchangeable, and any of our examples will turn out to

be such an E_N -extrinsic functional. Moreover, we will see that the Euclidean way to express these functionals gives us an approximate extrinsic access to this kind of intrinsic functionals.

4.1 Tangential Derivatives, Gradients and Hessians

In our setting of ESMs, we have to build two bridges to obtain a suitable tangential calculus in terms of Euclidean calculus in the ambient space: One extending functions from the ESM into the ambient space, and one that makes the calculus model in the ambient space independent of that very extension. The first bridge is already built by our knowledge about foliations of the ambient space and the extensions based on them, particularly the normal foliation and normal extension. The second bridge is now achieved straightforwardly: We first take an arbitrary but suitably smooth extension F of a function $f \in C^2(M)$ into tubular neighbourhood $U(M)$ and get its differential. Of course, this differential does not have a reasonable meaning within M itself: Simple calculus shows that if $F : \mathbb{R}^2 \rightarrow \mathbb{R}$ with $F(x, y) = x$ is restricted to the unit circle S^1 , then the result is far from being linear as a function of S^1 . Instead, we rather have that $F|_{S^1}$ is $t \mapsto \cos(t)$ for some $t \in [0, 2\pi[$. But as soon as we project the result onto the tangent space $T_x M$ at each $x \in M$, we get precisely what we would expect from a gradient, just w.r.t. the ESM — in case of our example, the tangent of $(x, y) = (\cos t, \sin t)$ is $(-\sin t, \cos t)$ and the Euclidean Jacobian of F is $(1, 0)$, so we obtain precisely the expected $t \mapsto -\sin t$ as the intrinsic differential.

4.1.1 Definition and Basic Properties

With the initial example in mind, we will now express the intrinsic derivative as the projection of the derivative onto the tangent space — first with a rather abstract definition, but we will soon be able to give a more convenient expression for the concept⁽¹⁾:

4.1 Definition For any $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ and differentiable function $f : M \rightarrow \mathbb{R}$ extended to neighbourhood $U(M)$ as $F : U(M) \rightarrow \mathbb{R}$ with $f = F|_M$ we define the *tangential derivative* operator D_M via the Euclidean derivative operator D as

⁽¹⁾In [36], the same operator is introduced for codimension one. There, it is also proven for the case of codimension one that this operator coincides with the definition for Riemannian derivatives in terms of parameterisations and parameter spaces, and the proof uses no features of the codimension, so it generalises naturally to higher codimension. We omit the details here, as this way of expressing the tangential derivative plays no relevant role for us. For a short explanation of the more general Riemannian setting, where the concepts introduced here appear with label “Riemannian” instead of “tangential”, see Appendix 9.3.

$$D_M f(x) = \Pi_{T_x^t M} DF(x),$$

where T_x^t is the *cotangent space* and Π_V is the orthogonal projection onto a vector subspace V of \mathbb{R}^d . Accordingly, we define the *tangential gradient* as

$$\nabla_M f(x) := \Pi_{T_x M} \nabla F(x).$$

4.2 Remark: (1) Obviously, this definition coincides with the classical Euclidean directional derivative of the extension for any tangent direction by definition. By this observation one can directly conclude that it is independent of the extension. (2) For the tangential gradient (and correspondingly for the differential), one can in particular use the equivalent formulation

$$\nabla_M f(x) := \nabla F(x) - \Pi_{N_x M} \nabla F(x).$$

This is interesting in practice whenever the codimension κ is smaller than the dimension k , as the projection onto the (co-)normal space is easier to calculate in this case. Since that is the usual situation we are going to face in future (because our prime objective will be surfaces in \mathbb{R}^3), it is also the formulation we will use most often. Additionally, it has certain useful implications that shall be investigated further in the course of this section, and it is more convenient in proving them.

The following technical lemma will now give us a more practical form of this tangential gradient for our future treatment:

4.3 Lemma *For any pointwise orthonormal frame $N(x) = (v^1(x), \dots, v^k(x))$ of the normal space $N_x M$ to $x \in M$, the tangential gradient can be expressed in the form*

$$\nabla_M f(x) := \nabla F(x) - \sum_{i=1}^k (D_{v^i} F)(x) v^i(x).$$

Therein, $D_{v^i} F$ is the directional derivative in direction of $v^i(x)$.

Proof: We write the projection from our definition in the standard version for given orthonormal frame:

$$\Pi_{N_x M}(\cdot) = \sum_{i=1}^k \langle v^i(x), \cdot \rangle v^i(x).$$

The projection is well-known to be independent of the choice of the frame, and we can apply the resulting vector to $\nabla F(x)$ and conclude

$$\nabla_M f(x) = \nabla F(x) - \sum_{i=1}^k \langle v^i(x), \nabla F(x) \rangle v^i(x) = \nabla F(x) - \sum_{i=1}^k (D_{v^i} F)(x) v^i(x).$$

□

4.4 Remark: By Lemma 2.16 we know that there is a locally smooth map N that assigns a normal frame $N(x) = (v^1(x), \dots, v^k(x))$ to any $x \in M$, and this map is in particular also smooth as a function in the ambient space. Using this, the notation of tangential gradient can be simplified further, as we have thereby locally

$$\nabla_M f(x) = \nabla F(x) - N(x) \cdot \nabla_N F(x).$$

Therein, we understand $\nabla_N F(x)$ as $\nabla_N F(x) = (D_{v^1} F(x), \dots, D_{v^k} F(x))^t$.

Things become more involved for the second order case: The concept of tangential derivative generalises naturally to higher orders by concatenated application. Most important to us will be the tangential derivative of second order, which gives us a *tangential Hessian*⁽²⁾:

4.5 Definition Let $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ and let $f : M \rightarrow \mathbb{R}$ be a twice continuously differentiable function extended to twice continuously differentiable $F : U(M) \rightarrow \mathbb{R}$ such that $f = F$ on M . Then we define for $x \in M$ the *tangential Hessian* matrix as

$$H_f^M(x) := D_M \nabla_M f(x)$$

and the corresponding pointwise bilinear form $H_f^M(x)(\cdot, \cdot)$ on $\mathbb{R}^d \times \mathbb{R}^d$ by

$$H_f^M(x)(v, w) = v^t H_f^M(x) w.$$

4.6 Remark: Note that the tangential Hessian is no longer just the restriction of the Euclidean Hessian of F to the tangent space, in contrast to the gradient: In our initial example, the second order differential of $F(x, y) = x$ vanishes everywhere, but clearly the second order differential of its restriction to the unit circle is $-\cos t$ for some t . In fact, $H_f^M(x)(\cdot, \cdot)$ of a C^2 -function F is in general not even a symmetric bilinear form on all of \mathbb{R}^d (cf. [29, Subs. 8.5.3]).

We now sum up a collection of useful properties for the tangential Hessian. Most importantly, we will be interested in the properties of $H_f^M(x)$ as a pointwise bilinear map on the respective tangent space $T_x M$. In particular, we find that for the

⁽²⁾We obtain this by tangential differentiation of a tangential gradient, or more generally speaking by covariant differentiation of a Riemannian gradient, cf. [7, Sect. 5.4] for a description of the concept in the setting of submanifolds of manifolds. Note in particular that the respective operations reduce to the Euclidean ones in the manifold \mathbb{R}^d ! For a short explanation of the more general Riemannian setting, see Appendix 9.3.

normal extension⁽³⁾, the tangential Hessian coincides with the Euclidean Hessian as a bilinear map on $T_x M$ at any $x \in M$.

4.7 Theorem *Let $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$, let $F \in C^2(U(M), \mathbb{R})$ and let $f = F|_M$. Then there are constants $c_1, c_2 > 0$ depending on M , but independent of F or f , such that for any $x \in M$*

$$\|\nabla_M f(x) - \nabla F(x)\|_2 \leq c_1 \max_{\substack{v \in N_x M \\ \|v\|_2 = 1}} |D_v F(x)|$$

and for any $v, w \in T_x M$

$$|H_f^M(x)(v, w) - H_F(x)(v, w)| \leq c_2 \max\{|D_v F(x)| \cdot \|v\|_2 \cdot \|w\|_2 : v \in N_x M, \|v\|_2 = 1\}.$$

Proof: The first result is a direct consequence of Lemma 4.3, so we only work on the second here: We conclude immediately from the definition of the tangential Hessian and Remark 4.4 that locally

$$H_f^M(v, w) = v^t H_f w - v^t D(N \cdot \nabla_N F) w. \quad (4.7.1)$$

Then we demand without restriction a coordinate system where the first k coordinates correspond to tangent and the last κ coordinates correspond to normal basis vectors. Now we take a closer look at $D(N \cdot \nabla_N F)$ and decompose it as

$$D \left(\sum_{i=1}^K (D_{v^i} F) v^i \right) = \sum_{i=1}^K D((D_{v^i} F) v^i).$$

We restrict ourselves now to one coordinate ℓ for $1 \leq \ell \leq d$ and look at just $\partial_\ell((D_{v^i} F) v^i)$ closer for arbitrary v^i . As each $(D_{v^i} F) v^i$ still has multiple entries, we restrict us further to just one $(D_{v^i} F) N_{ij}$. There we find by the product rule

$$\partial_\ell((D_{v^i} F) N_{ij}) = (\partial_\ell(D_{v^i} F)) N_{ij} + (D_{v^i} F) (\partial_\ell N_{ij}).$$

Reinserting this into $\partial_\ell((D_{v^i} F) v^i)$ we obtain

$$\partial_\ell((D_{v^i} F) v^i) = (\partial_\ell(D_{v^i} F)) v^i + (D_{v^i} F) (\partial_\ell v^i).$$

Then we get for the overall $D(N \cdot \nabla_N F)$ that

$$D(N \cdot \nabla_N F) = \sum_{i=1}^K v^i \cdot D(D_{v^i} F) + \sum_{i=1}^K (D_{v^i} F) (D v^i).$$

Multiplication of this by an arbitrary cotangent v^t from the left and by an arbitrary

⁽³⁾Actually, this holds for any orthogonal extension.

tangent w from the right will annihilate the first sum. This in mind, we reinsert into (4.7.1) and obtain

$$H_f^M(x)(v, w) = v^t H_f(x) w - v^t \left(\sum_{i=1}^{\kappa} (D_{v^i} F)(x) (Dv^i)(x) \right) w.$$

Since N can be presumed to be C -bounded by Lemma 2.16, and hence the bilinear form induced by $Dv^i(x)$ is bounded for any $i = 1, \dots, \kappa$, we can deduce that

$$\left| v^t D \left(N \cdot \frac{\partial F}{\partial N} \right) w \right| \leq \max_{1 \leq i \leq d-q} |D_{v^i} F(x)| \cdot \sum_{i=1}^{\kappa} |v^t Dv^i(x) w| \leq c_2 \max_{\substack{v \in N_x M \\ \|v\|_2 = 1}} |D_v F(x)| \cdot \|v\|_2 \cdot \|w\|_2.$$

Hence, we obtain the desired result. \square

This theorem gives us an approximate handling of second order tangential derivatives just as approximate Euclidean derivatives whenever the directional derivative in normal directions is small. In particular, the correspondence between tangential and Euclidean derivative is *exact* whenever the normal derivative vanishes — which is the case if the extension was obtained by the normal extension operator. This fact is so important to us that we repeat it here as a statement of its own⁽⁴⁾:

4.8 Corollary *As a bilinear map of the tangent space, the tangential Hessian bilinear map $H_f^M(x)(\cdot, \cdot) : T_x M \times T_x M \rightarrow \mathbb{R}$ does coincide with the standard Hessian bilinear map $H_{\bar{F}}(x)(\cdot, \cdot) : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}$ of normal extension \bar{F} of f , so*

$$H_f^M(x)(v, w) = H_{\bar{F}}(x)(v, w) \quad \forall v, w \in T_x M.$$

With these newly defined first and second order tangential derivatives, we can also ask for further operators on these, and we shall give at least one example here: the *Laplace-Beltrami operator* Δ_M . It comes easily now, and we directly give a suitable definition (cf. e.g. [57, pp. 359], [83, p. 28]):

4.9 Definition Let $M \in \mathbb{M}_{bd}^k(\mathbb{R}^d)$. Then the *Laplace-Beltrami operator* Δ_M is defined for arbitrary $f \in C^2(M)$ as the trace of the Hessian, so for $H_f^M(x)$ with entries $h_{ij}^f(x)$ for $i, j = 1, \dots, d$ it holds

$$\Delta_M f(x) = \sum_{i=1}^d h_{ii}^f(x).$$

4.10 Remark: We can define a tangential divergence operator div_M for a tangent vector field $v : M \rightarrow TM$ with $v(x) = (v_1(x), \dots, v_d(x))^t$ as

⁽⁴⁾The statement of this corollary is also given in [29, Subs. 8.5.3] for the case of codimension one, but in a more "differential geometric style".

$$\operatorname{div}_M \mathbf{v} = \sum_{i=1}^d (D_M \mathbf{v}_i)_i.$$

Then we obtain the tangential Laplacian simultaneously as the divergence of the gradient field.

In case of an extension based on an orthogonal foliation, we directly obtain the following important simplification of that definition as a consequence of Corollary 4.8 and the fact that the trace of a bilinear form is an invariant under orthogonal basis transformations⁽⁵⁾:

4.11 Corollary *Let $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$. For any $x \in M$ it holds with the normal extension operator E_N that*

$$\Delta_M f(x) = \Delta(E_N f)(x),$$

where Δ is the standard Laplacian operator in the ambient space $U(M)$. For an arbitrary tangent frame $T(x) = (\tau^1(x), \dots, \tau^k(x))$ it holds

$$\Delta_M f(x) = \Delta_T(E_N f)(x) := \sum_{i=1}^k D_{\tau^i}^2(E_N f)(x).$$

For an arbitrary smooth extension F of f still holds

$$|\Delta_M f(x) - \Delta_T(F)(x)| \leq c \max_{\substack{v \in N_x M \\ \|v\|_2 = 1}} |D_v F(x)|.$$

With tangential versions of the gradient and the Laplacian, we can further state a tangential version of Green's theorem (cf. [18, Th. 17], [83, Cor. 46, p. 382]):

4.12 Proposition — Tangential Green's Theorem —

Let $F \in C^2(U(M))$ and $f = F|_M$. If M has no boundary, then it holds

$$\int_M f \Delta_M f = - \int_M \langle \nabla_M f, \nabla_M f \rangle$$

and if M has boundary $\Gamma \neq \emptyset$, then it holds

$$\int_M f \Delta_M f = - \int_M \langle \nabla_M f, \nabla_M f \rangle + \int_\Gamma f D_\nu f,$$

where $D_\nu f$ is the directional derivative in the direction of the relative outer normal ν of Γ relative to M .

4.13 Remark: In Appendix 9.3, a short introduction into the more general Rie-

⁽⁵⁾Again, this result was already used and presented in [36] for codimension one, but without the general context of Hessians we provided here.

mannian setting is given. There we also comment briefly on the relation between our definitions and further common ways to express these terms, in particular in terms of parameterisations.

4.1.2 Intrinsic Characterisation of Sobolev Spaces

Now we have a closer look at the tangential Hessian itself and deduce the important property of invariance under rotation of the specific tangent frame. This will give us the key to derive an intrinsic definition of Sobolev norms:

4.14 Lemma 1. Let $g : \Omega \subseteq \mathbb{R}^d \rightarrow \mathbb{R}$ be twice continuously differentiable and $x \in \Omega$. Then the quantity

$$\sum_{i,j=1}^d \left| \frac{\partial^2 g}{\partial v^i \partial v^j}(x) \right|^2$$

is independent of the specific choice of an orthonormal frame v^1, \dots, v^d of \mathbb{R}^d .

2. If $\tilde{F} = E_N f$ is the normal extension of some function $f \in C^2(M, \mathbb{R})$ for ESM M into ambient neighbourhood $U(M)$, $x \in M$ and $\tau^1(x), \dots, \tau^k(x)$ is an arbitrary orthonormal frame of $T_x M$, then we have

$$\sum_{i,j=1}^k |H_f^M(\tau^i, \tau^j)|^2 = \sum_{i,j=1}^k |H_{\tilde{F}}(\tau^i, \tau^j)|^2.$$

Again, this relation is independent of the specific choice of the tangent frame and invariant under rotation (in the tangent space) of that basis on either side.

3. If v^1, \dots, v^k is another basis of the tangent space, then we have for suitable constants c_1, c_2 depending on the basis that

$$c_1 \sum_{i,j=1}^k |H_f^M(v^i, v^j)|^2 \leq \sum_{i,j=1}^k |H_f^M(\tau^i, \tau^j)|^2 \leq c_2 \sum_{i,j=1}^k |H_f^M(v^i, v^j)|^2.$$

If the basis frame $Y(x) = (v^1, \dots, v^k)$ is continuous in a neighbourhood of $x \in M$, then the constants depend continuously on $x \in M$. If $Y \circ \psi$ is C -bounded in parameter space ω of the inverse atlas of M and its spectrum is bounded from below by $\varepsilon > 0$, then all constants are globally bounded on $\psi(\omega)$.

Proof: 1. Obvious, since it is the squared Frobenius matrix-norm $\|\cdot\|_F$, which in turn is a rewritten Euclidean norm on \mathbb{R}^{d^2} .

2. and 3. can be deduced from a common start: Let $T(x) = (\tau^1(x), \dots, \tau^k(x))$ be an orthonormal frame of the tangent space and $Y(x) = (v^1(x), \dots, v^k(x))$ be another, not necessarily orthonormal, frame. By standard linear algebra, there is $\Lambda_{Y,T} \in \mathbb{R}^{k \times k}$ such that $T = Y \Lambda_{Y,T}$, and in the same way, there is $\Lambda_{T,Y}$ such that $Y = T \Lambda_{Y,T}$.

Both $\Lambda_{Y,T}$ and $\Lambda_{Y,T}$ depend locally continuous on $x \in \mathbb{M}$. Now it holds with the submultiplicativity of the Frobenius matrix-norm and Corollary 4.8 that

$$\begin{aligned} \sum_{i,j=1}^k |H_f^{\mathbf{M}}(\tau^i, \tau^j)|^2 &= \|T^t H_{\overline{F}} T\|_F^2 = \|\Lambda_{Y,T}^t Y^t H_{\overline{F}} Y \Lambda_{Y,T}\|_F^2 \\ &\leq \|\Lambda_{Y,T}\|_F^2 \|Y^t H_{\overline{F}} Y\|_F^2 \|\Lambda_{Y,T}\|_F^2 = \|\Lambda_{Y,T}\|_F^4 \sum_{i,j=1}^k |H_f^{\mathbf{M}}(\mathfrak{v}^i, \mathfrak{v}^j)|^2, \end{aligned}$$

In the same way one obtains

$$\sum_{i,j=1}^k |H_f^{\mathbf{M}}(\mathfrak{v}^i, \mathfrak{v}^j)|^2 \leq \|\Lambda_{T,Y}\|_F^4 \sum_{i,j=1}^k |H_f^{\mathbf{M}}(\tau^i, \tau^j)|^2,$$

whereby one directly deduces the third claim. To deduce the second, we can assume that Y is now also orthonormal. In that case, both $\Lambda_{Y,T}$ and $\Lambda_{Y,T}$ are orthogonal matrices, as one easily verifies. Thereby the second claim is also fairly obvious, as the Frobenius norm remains unaffected by orthogonal transforms on either side. We shall now just give a short argument for $\Lambda_{Y,T}$ being orthogonal: We take the normal frame N and enhance both tangent frames to global frames, (T, N) and (Y, N) . Filling up $\Lambda_{Y,T}$ by zeros on the left and below, and by an κ unit matrix in the lower right, we can deduce

$$I_d = (T, N)(T, N)^t = (Y, N) \begin{pmatrix} \Lambda_{Y,T} & O_{k \times \kappa} \\ O_{\kappa \times k} & I_{\kappa} \end{pmatrix} (T, N)^t,$$

which gives in turn

$$(Y, N)^t (T, N) = \begin{pmatrix} \Lambda_{Y,T} & O_{k \times \kappa} \\ O_{\kappa \times k} & I_{\kappa} \end{pmatrix},$$

and as the left is orthogonal, so is the right. \square

The next theorem gives us an intrinsic characterisation of the space $H^2(\mathbb{M})$ independent of any inverse atlas, but equivalent to the definition we have previously introduced. But before we come to that we make one more important definition:

4.15 Definition Let $\mathbb{M} \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ and $f \in H^2(\mathbb{M})$. Then we define the *Hessian energy* $\epsilon_H(f, f)^{(6)}$ by

$$\epsilon_H(f, g) := \int_{\mathbb{M}} \epsilon_H(f, g),$$

where in turn

$$\epsilon_H(f, g) := \sum_{i,j=1}^k H_f^{\mathbf{M}}(\tau^i, \tau^j) \cdot H_g^{\mathbf{M}}(\tau^i, \tau^j)$$

⁽⁶⁾The letters ϵ and ϵ are a script- or crescent-shaped variant of epsilon that is used here to avoid any confusion with our extension operators. It was particularly common in byzantine scripts, and still is in coptic.

for $(\tau^1, \dots, \tau^k) = (\tau^1(x), \dots, \tau^k(x))$ an arbitrary orthonormal frame of the tangent space $T_x M$ at any $x \in M$.

4.16 Theorem *The chart based definition of the norms $\|f\|_{H^1(M)}, \|f\|_{H^2(M)}$ from Definition 2.24 for any finite C-bounded Lipschitz inverse atlas $\mathbb{A}_M \in \Pi(M)$ are equivalent to the following definitions of norms:*

$$\|f\|_{H_T^1(M)}^2 := \int_M |f|^2 + \int_M \|\nabla_M f\|_2^2 \quad \|f\|_{H_T^2(M)}^2 := \|f\|_{H_T^1(M)}^2 + \epsilon_H(f, f).$$

Proof: Since we have a finite inverse atlas \mathbb{A}_M , we restrict ourselves here to one pair (ψ, ω) from \mathbb{A}_M , and we understand the norms $\|f\|_{H_T^1(M)}$ and $\|f\|_{H_T^2(M)}$ in the Sobolev case as metric closures of the smooth functions. Then by the transformation law

$$c_1 \|f \circ \psi\|_{L_2(\omega)}^2 \leq \int_{\psi(\omega)} |f|^2 \leq c_2 \|f \circ \psi\|_{L_2(\omega)}^2.$$

By considering additionally the chain rule and the fact that $D\psi$ maps into a basis of the tangent space and this map is C-bounded⁽⁷⁾, we can further deduce that

$$c_1 \int_{\omega} |\nabla(f \circ \psi)|^2 \leq \int_{\psi(\omega)} |\nabla_M f|^2 \leq c_2 \int_{\omega} |\nabla(f \circ \psi)|^2.$$

This comes as follows: The change of basis that the transition from old basis $\tau^1, \dots, \tau^k, \nu^1, \dots, \nu^k$ to the new basis $\frac{\partial \psi}{\partial x_1}, \dots, \frac{\partial \psi}{\partial x_k}, \nu^1, \dots, \nu^k$ invokes (and vice versa) has C-bounded entries by definition of ψ and bounded absolute values of its spectrum within some interval $[a, b]$ for $0 < a \leq b < \infty$, and thus all constants are globally bounded. So we need to take care about the second order terms only. There, we have for arbitrary coordinate directions x_i, x_j with respect to ω that by the chain rule

$$\frac{\partial^2 (\vec{F} \circ \psi)}{\partial x_i \partial x_j} = \left(\frac{\partial \psi_1}{\partial x_i}, \dots, \frac{\partial \psi_d}{\partial x_i} \right) \cdot H_{\vec{F}}(\psi(x)) \cdot \left(\frac{\partial \psi_1}{\partial x_j}, \dots, \frac{\partial \psi_d}{\partial x_j} \right)^t + \sum_{\ell=1}^d \partial_\ell \vec{F} \frac{\partial^2 \psi_\ell}{\partial x_i \partial x_j}.$$

By definition, the set

$$\left\{ \partial_i \psi := \left(\frac{\partial \psi_1}{\partial x_i}, \dots, \frac{\partial \psi_d}{\partial x_i} \right)^t \right\}_{i=1}^k$$

forms a pointwise basis of the tangent space, and the corresponding basis transform has a bounded spectrum due to C-boundedness by conception of \mathbb{A}_M . So with the third statement of the last lemma we can deduce that

⁽⁷⁾By conception of \mathbb{A}_M , and this is also a consequence of appendix Theorem 9.6.

$$\begin{aligned}
\left(\frac{\partial^2 (\vec{F} \circ \psi)}{\partial x_i \partial x_j} \right)^2 &\leq \left(|(\partial_i \psi)^t \cdot H_{\vec{F}}(\psi(x)) \cdot (\partial_j \psi)| + \left| \sum_{\ell=1}^d \partial_\ell \vec{F} \frac{\partial^2 \psi_\ell}{\partial x_i \partial x_j} \right| \right)^2 \\
&\leq c \left| (\partial_i \psi)^t \cdot H_{\vec{F}}(\psi(x)) \cdot (\partial_j \psi) \right|^2 + c \left| \sum_{\ell=1}^d \partial_\ell \vec{F} \frac{\partial^2 \psi_\ell}{\partial x_i \partial x_j} \right|^2 \\
&\leq c \epsilon_H(f, f) + c \langle \nabla_M f, \nabla_M f \rangle^2,
\end{aligned}$$

where we used further that $\nabla_M f = \nabla \vec{F}$. Thereby we can deduce that

$$\int_{\omega} \sum_{i,j=1}^k \left(\frac{\partial^2 (\vec{F} \circ \psi)}{\partial x_i \partial x_j} \right)^2 \leq c \|f\|_{H_1^2(M)}^2,$$

which gives one part of the required inequality. For the other, we argue by contradiction: We assume that we have a sequence $(f_n)_{n \in \mathbb{N}}$ of functions with corresponding $\vec{F}_n = E_N f_n$ such that $\|f_n\|_{H_1^2(M)}^2 \geq 1$ but

$$\|f_n\|_{H^2(M)} < \frac{1}{n} \quad \forall n \in \mathbb{N}.$$

Without restriction, we demand these functions to be smooth. Then we can directly deduce from the known equivalence of $\|f\|_{H^1(M)}$ and $\|f\|_{H_1^1(M)}$, and from Sobolev embeddings, that also

$$\|f_n\|_{H_1^1(M)} < c \frac{1}{n},$$

so again it boils down to the second order term only. There we see now that in particular

$$\int_{\omega} \left(\frac{\partial^2 (\vec{F}_n \circ \psi)}{\partial x_i \partial x_j} \right)^2 < \frac{1}{n}.$$

On the other hand, we can deduce that with $\partial_{ij} \psi := \left(\frac{\partial^2 \psi_1}{\partial x_i \partial x_j}, \dots, \frac{\partial^2 \psi_d}{\partial x_i \partial x_j} \right)^t$ we have by the chain rule

$$\begin{aligned}
\left(\frac{\partial^2 (\vec{F}_n \circ \psi)}{\partial x_i \partial x_j} \right)^2 &= \left((\partial_i \psi)^t H_{\vec{F}_n}(\psi(x)) (\partial_j \psi) + \langle \partial_{ij} \psi, \nabla_M f_n \rangle \right)^2 \\
&= \left((\partial_i \psi)^t H_{\vec{F}_n}(\psi(x)) (\partial_j \psi) \right)^2 + \langle \partial_{ij} \psi, \nabla_M f_n \rangle^2 \\
&\quad + 2 \left((\partial_i \psi)^t H_{\vec{F}_n}(\psi(x)) (\partial_j \psi) \right) \cdot \langle \partial_{ij} \psi, \nabla_M f_n \rangle \\
&\geq \left((\partial_i \psi)^t H_{\vec{F}_n}(\psi(x)) (\partial_j \psi) \right)^2 \\
&\quad - 2 \left| \left((\partial_i \psi)^t H_{\vec{F}_n}(\psi(x)) (\partial_j \psi) \right) \cdot \langle \partial_{ij} \psi, \nabla_M f_n \rangle \right|.
\end{aligned}$$

Integrating over both after summing over all i, j gives

$$\begin{aligned}
\frac{1}{n} &> \int_{\omega} \sum_{i,j=1}^k \left(\frac{\partial^2 (\vec{F}_n \circ \psi)}{\partial x_i \partial x_j} \right)^2 \\
&\geq \int_{\omega} \sum_{i,j=1}^k \left((\partial_i \psi)^t H_{\vec{F}_n}(\psi(x)) (\partial_j \psi) \right)^2 \\
&\quad - 2 \int_{\omega} \sum_{i,j=1}^d \left| \left((\partial_i \psi)^t H_{\vec{F}_n}(\psi(x)) (\partial_j \psi) \right) \cdot \langle \partial_{ij} \psi, \nabla_M f_n \rangle \right|.
\end{aligned}$$

On the other hand, Hölder's inequality gives that

$$\begin{aligned}
&\sum_{i,j=1}^k \int_{\omega} \left| \left((\partial_i \psi)^t H_{\vec{F}_n}(\psi(x)) (\partial_j \psi) \right) \cdot \langle \partial_{ij} \psi, \nabla_M f_n \rangle \right| \\
&\leq c \sum_{i,j=1}^k \left(\int_{\omega} \left((\partial_i \psi)^t H_{\vec{F}_n}(\psi(x)) (\partial_j \psi) \right)^2 \right)^{\frac{1}{2}} \cdot \left(\int_{\omega} \langle \partial_{ij} \psi, \nabla_M f_n \rangle^2 \right)^{\frac{1}{2}} \\
&\leq c \sum_{i,j=1}^k \left(\int_{\omega} \left((\partial_i \psi)^t H_{\vec{F}_n}(\psi(x)) (\partial_j \psi) \right)^2 \right)^{\frac{1}{2}} \cdot \left(\int_{\omega} \langle \partial_{ij} \psi, \partial_{ij} \psi \rangle \langle \nabla_M f_n, \nabla_M f_n \rangle \right)^{\frac{1}{2}} \\
&\leq c \|f_n\|_{H^2} \|f_n\|_{H^1} \leq c \cdot \frac{1}{n}.
\end{aligned}$$

Inserting this gives

$$\frac{1}{n} > \int_{\omega} \sum_{i,j=1}^k \left((\partial_i \psi)^t H_{\vec{F}_n}(\psi(x)) (\partial_j \psi) \right)^2 - c \cdot \frac{1}{n},$$

and so we deduce that

$$\int_{\omega} \sum_{i,j=1}^k \left((\partial_i \psi)^t H_{\vec{F}_n}(\psi(x)) (\partial_j \psi) \right)^2 \leq c \cdot \frac{1}{n}.$$

But this produces a contradiction, as we can bound

$$\int_{\omega} \sum_{i,j=1}^k \left((\tau^i)^t H_{\vec{F}_n}(\psi(x)) (\tau^j) \right)^2 \leq c \int_{\omega} \sum_{i,j=1}^d \left((\partial_i \psi)^t H_{\vec{F}_n}(\psi(x)) (\partial_j \psi) \right)^2$$

and thus we would have

$$1 \leq \|f_n\|_{H^2_1(M)} < c \frac{1}{n} \quad \forall n \in \mathbb{N}.$$

□

4.2 Unisolvency in Tangential Calculus

Since now a second order tangential derivative is available, we can ask ourselves if there are also functions in $H^2(M)$ that have *optimal* second order energy under suitable constraints, in particular interpolation constraints on some finite set $\Xi \in M$. That is, if there is a function $f^* \in H^2(M)$ that interpolates given function values at the points of a finite set $\Xi \subseteq M$ such that f^* minimises

$$E_H(f, f) = \int_M \sum_{i,j=1}^k |H_f^M(\tau^i, \tau^j)|^2.$$

In \mathbb{R}^d , it is well-known that this is possible under some mild conditions on Ξ : As long as Ξ is *unisolvent* for the linear polynomials $P^2(\mathbb{R}^d)$, so there is no linear polynomial other than the zero function that vanishes in all points, the minimum exists, and it is even explicitly known (cf. [105]). And the check for unisolvency is not too hard, either: Ξ is unisolvent for $P^2(\mathbb{R}^d)$ if and only if Ξ contains at least $d + 1$ points that are not part of a common affine subspace of \mathbb{R}^d (cf. [105]).

We hope that a similar concept will also hold on more general ESMs. So we ask ourselves what amount and distribution of points Ξ is necessary to determine that the kernel of the second order tangential derivative operator is trivial if we demand $f(\xi) = 0$ for all $\xi \in \Xi$.

4.17 Remark: In the course of this section, we treat only the case of C^2 -functions on M . However, this generalises directly to the distributional case: To deduce this, it suffices to verify that any function in the kernel of $E_H(f, f)$ actually has to be twice continuously differentiable. To this end, we first conclude that whenever the quadratic form $E_H(f, f)$ vanishes for a function $f \in H^2(M)$, then necessarily $\Delta_M f$ will vanish as well. This implies that a function from the kernel is necessarily a *harmonic function* on M . And one deduces from the regularity theory of elliptic PDEs (cf. [83, Th. 67, p. 281]) that any of these functions has to be C^∞ in case of a smooth M !

A suitable condition for points on an ESM M is easily determined if $M \in \mathbb{M}_{\text{cp}}^k(\mathbb{R}^d)$, so is compact and thus has no boundary. It comes by application of the tangential version of Green's theorem:

4.18 Theorem *Let $M \in \mathbb{M}_{\text{cp}}^k(\mathbb{R}^d)$. Then any function $f \in C^2(M)$ whose tangential Hessian vanishes identically on M is constant, and the same holds true if $\Delta_M f$ vanishes identically.*

Proof: With all intrinsic second derivatives vanishing, so must in particular the Laplace-Beltrami of f . So we are in the second situation and have there that

$$\Delta_M f(x) = 0 \quad \forall x \in M.$$

Then we employ Green's theorem to obtain

$$0 = \int_M f \Delta_M f = - \int_M \langle \nabla_M f, \nabla_M f \rangle \leq 0.$$

Consequently $\nabla_M f = 0$ everywhere, and therefore f must be constant. \square

So whenever M is compact, we have that one single point suffices to determine the kernel as the zero function. However, we can easily find that when M has a boundary, the conditions have to be more elaborate: Even a domain in \mathbb{R}^d suffices as a counterexample.

Of course, we could employ boundary conditions, for example Neumann conditions, to achieve the same result just as we did above. On the other hand, why should one use boundary conditions if there is no need for them? So we would like to have a comparable result by simply considering a finite discrete set of points like in the Euclidean case. This hope and the correspondence to the common Euclidean case justifies the following definition:

4.19 Definition For $M \in \mathcal{M}_{\text{bd}}^k(\mathbb{R}^d)$, a set $\Xi \subseteq M$ of discrete points is said to be D_M^ℓ -*unisolvent* if the only function from the kernel of the ℓ th order tangential derivative operator that vanishes at all points of Ξ is the constant zero function.

4.20 Remark: Obviously, any superset of some D_M^ℓ -unisolvent set is D_M^ℓ -unisolvent itself.

A suitable condition for unisolvency in the case *with* boundary is easily determined for curves: There is an obvious one-to-one correspondence between the tangential derivative of order ℓ of a smooth curve γ (seen as an ESM in its own right) and the derivative of order ℓ on the parameter interval for an arc length parameterisation γ of the curve γ : they effectively coincide, so

$$D_\gamma^\ell f(x) = D^\ell(f \circ \gamma)(\tilde{x}), \quad x = \gamma(\tilde{x}), \quad \tilde{x} \in I$$

for the arc length parameterisation $\gamma : I \rightarrow \mathbb{R}^d$. So for any curve, two points will suffice for the case $\ell = 2$, and for a closed curve, even one point will do the job.

4.21 Conclusion On an ESM γ that is an open curve, any set of at least ℓ points is D_M^ℓ -unisolvent.

4.2.1 Unisolvency and Curvature

Surprisingly, there is a comparably simple characterisation of arbitrary ESMs of dimension $k \geq 2$ that admit no other functions with vanishing Hessian than the

constant functions even if they have nonempty boundary. If in particular $k = 2$, then it turns out that only a surface whose Gaussian curvature⁽⁸⁾ does vanish identically can ever have nonconstant functions with vanishing Hessian. That is, any surface where this kernel is nontrivial must necessarily be a *developable surface*. We will deduce this condition now by a sequence of suitable arguments.

But before we come to that, we need a handful of appropriate definitions, stated here in some specialised version but based on the general Riemannian setting. They can be found for example in [9, Ch. 1], [34, Ch. 4] and [51, Ch. II and III], on which we shall rely here:

4.22 Definition Let $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$. Let $\Gamma(M)$ be the set of all smooth tangent vector fields on M .

1. Let $u \in \Gamma(M)$. Let $u(y) := (u_1(y), \dots, u_d(y))^t$. Then we define the (tangential) *covariant derivative* $\nabla_v u(y)$ of u in y along a vector field $v \in \Gamma(M)$ by

$$\nabla_v u(y) = ((D_M u_1(y))v(y), \dots, (D_M u_d(y))v(y))^t.$$

2. We call $u \in \Gamma(M)$ a *parallel vector field* if $\nabla_v u(y) = 0$ for any $y \in M$ and any $v \in \Gamma(M)$.
3. We call $u \in \Gamma(M)$ an *integrable vector field* if each curve integral exists and does not depend on the actual path from its start to its end.

4.23 Example: The gradient of any function with vanishing Hessian is by definition of parallel vector fields such a parallel vector field: If its tangential Hessian vanishes, then any covariant derivative of the gradient along any vector field will vanish in particular. Further, any such field is integrable according to the above definition.

We begin now with a couple of subsequent lemmata that provide us with useful facts about covariant derivatives and parallel vector fields:

4.24 Lemma Let $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$, let $y \in M$ and let $u, v, w, x \in \Gamma(M)$. Then the following rules hold locally around y :

1. $\nabla_{\eta x + w} u = \eta \nabla_x u + \nabla_w u$ for any $\eta \in C^\infty(M)$.
2. $\nabla_w (\alpha u + v) = \alpha \nabla_w u + \nabla_w v$ for any $\alpha \in \mathbb{R}$.
3. $D_w \langle u, v \rangle = \langle \nabla_w u, v \rangle + \langle u, \nabla_w v \rangle$, where $D_w f := (D_M f)w$ for any $f \in C^\infty(M)$.

If w, x are globally linearly independent, all relations hold globally as well.

⁽⁸⁾We recall that in \mathbb{R}^3 the Gaussian curvature $K(x)$ of a surface M at a point $x \in M$ is the product of the principal curvatures $\kappa_1(x)$ and $\kappa_2(x)$. These are in turn the maximal and the minimal normal curvature in x taken over all geodesics through x .

Proof: The first two are direct consequences of the definition. The third is then also easily seen: By definition, the tangential derivative satisfies the product rule in the form

$$D_M(f \cdot g) = gD_M f + fD_M g.$$

Then we suppose that $u = (u_1, \dots, u_d)^t$ and $v = (v_1, \dots, v_d)^t$ and choose an arbitrary $i \in \{1, \dots, d\}$. We obtain

$$D_M(u_i v_i) = v_i D_M u_i + u_i D_M v_i,$$

and conclude by summation that

$$D_M \langle u, v \rangle = \sum_{i=1}^d v_i D_M u_i + \sum_{i=1}^d u_i D_M v_i.$$

Multiplication of both sums by w yields

$$D_w \langle u, v \rangle = \sum_{i=1}^d v_i (D_M u_i)w + \sum_{i=1}^d u_i (D_M v_i)w = \langle \nabla_w u, v \rangle + \langle u, \nabla_w v \rangle.$$

□

4.25 Lemma *Let $u, v \in \Gamma(M)$ be parallel vector fields. Then $\langle u, v \rangle$ is constant. In particular, $\langle u, u \rangle$ and thus $\|u\|_2$ are constant.*

Proof: By the product rule for covariant derivatives presented in the last lemma, it holds locally around an arbitrary $y \in M$ for any $x \in \Gamma(M)$ that does not vanish at y that

$$D_x \langle u(y), v(y) \rangle = \langle \nabla_x u(y), v(y) \rangle + \langle u(y), \nabla_x v(y) \rangle = 0 + 0 = 0.$$

Consequently, $\langle u(y), v(y) \rangle$ must be constant in a neighbourhood of y , and thus globally constant because M was (always) supposed to be connected. □

4.26 Lemma *Let u^1, \dots, u^ℓ be $\ell \leq k$ linearly independent parallel tangent vector fields on M . Then there is a positively oriented pointwise orthonormal frame for the ℓ -section σ_M^ℓ defined as $\sigma_M^\ell(x) := \text{span}(u^1(x), \dots, u^\ell(x)) \subseteq T_x M$. In particular, any system of linearly independent parallel vector fields consists of at most k vector fields. All such maximal systems yield the same section.*

Proof: Without restriction, we can $\|u^i\| = 1$, $i = 1, \dots, \ell$. Then we can apply Gram-Schmidt orthonormalisation in each point, whereby we obtain new vector fields $v^1 = u^1$ and for $\lambda = 2, \dots, \ell$

$$v^\lambda(x) = \sum_{i=1}^{\lambda-1} \langle u^\lambda(x), u^i(x) \rangle u^i(x).$$

Because of Lemma 4.25, any coefficient is constant over M . Moreover, it holds for any $\lambda = 2, \dots, \ell$

$$\begin{aligned}\langle v^\lambda, v^\lambda \rangle &= \left\langle \sum_{i=1}^{\lambda-1} \langle u^\lambda(x), u^i(x) \rangle u^i(x), \sum_{j=1}^{\lambda-1} \langle u^\lambda(x), u^j(x) \rangle u^j(x) \right\rangle \\ &= \sum_{i,j=1}^{\lambda-1} \langle u^\lambda, u^i \rangle \langle u^\lambda, u^j \rangle \langle u^i, u^j \rangle,\end{aligned}$$

which is again constant over M . So parallelity of the new vector fields is retained due to the \mathbb{R} -linearity of covariant derivatives. Finally, if we had another section ρ_M^ℓ spanned by fields w^1, \dots, w^ℓ such that at a point x_0 we have $\sigma_M^\ell(x_0) \neq \rho_M^\ell(x_0)$, then there is a field w^0 with $w^0(x_0)$ linearly independent of $v^1(x_0), \dots, v^\ell(x_0)$. As it is also parallel and vanishes nowhere, it has constant angle to any v^i . Thus w^0 is linearly independent to these fields and ℓ is not maximal. \square

This result tells us that we have a vector space structure on the parallel vector fields. Recalling that the gradient field of a function with identically vanishing tangential Hessian is parallel, we obtain the following result that gives us a construction method for functions with vanishing Hessian.

4.27 Theorem *Let $M \in \mathbb{M}_{\text{sd}}^k(\mathbb{R}^d)$ and $f \in C^2(M)$ be a nonconstant function with*

$$\mathcal{C}_H(f, f) = 0.$$

Let $\{u^1, \dots, u^\ell\}$ be a maximal linear independent set of integrable orthonormal parallel tangent vector fields. Then $\nabla_M f$ has a unique representation of the form

$$\nabla_M f = \sum_{i=1}^{\ell} \alpha_i u^i$$

with real coefficients $\alpha_1, \dots, \alpha_\ell$.

This result tells us in turn that the kernel of $\mathcal{C}_H(f, f)$ is a finite dimensional space. We can even deduce its dimension, which has to be $\ell + 1$. And we can explicitly construct any function in the kernel if the gradient and a single function value in a point ξ_0 is given: If $\xi \in M$ is another point and γ is a curve in M that contains ξ_0, ξ with arc-length L and arc-length parameterisation $\gamma : [0, L] \rightarrow M$ such that $\gamma(0) = \xi_0$ and $\gamma(L) = \xi$, then one obtains

$$f(\xi) = f(\xi_0) + \int_0^L \langle \nabla_M f(\gamma(t)), \gamma'(t) \rangle dt = f(\xi_0) + \sum_{i=1}^{\ell} \alpha_i \int_0^L \langle u^i(\gamma(t)), \gamma'(t) \rangle dt.$$

Due to the integrability of the "basis fields" u^1, \dots, u^ℓ , this is independent of the actual choice of χ and thus provides a well-defined expression that defines f .

4.28 Conclusion Let $M \in \mathbb{M}_{\text{sd}}^k(\mathbb{R}^d)$ and let $\{u^1, \dots, u^\ell\} \subseteq \Gamma(M)$ be a maximal linear independent system of integrable orthonormal parallel vector fields. Then any function $f \in C^2(M)$ whose tangential Hessian vanishes on M is determined up to a constant by integration of the vector fields $\{u^1, \dots, u^\ell\}$.

The question is now what values we can expect for ℓ . As one would expect, the answer depends on the actual shape of M : All values between 0 and k are possible, and for each choice there are representatives; one simply has to choose $M = \mathbb{S}^{k-\ell} \times I^\ell$ for an arbitrary open interval I and $\ell = 0, \dots, k$.

The actual value can be hard to determine for an arbitrary M , but we shall see soon that for a wide range of ESMs and in particular for all surfaces whose Gaussian curvature does not vanish identically, there are no such parallel fields. To accomplish this, we need some further definitions. Namely, we require some concepts of curvature for an ESM that give us the usual Gaussian curvature of standard differential geometry in particular (cf. [9, Ch. 1] and [34, Sect. 4.2/4.3]):

4.29 Definition Let $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$. For three vector fields $u, v, w \in \Gamma(M)$ we define the (tangential) *curvature tensor* $R_x^M(u, v)w$ of u, v and w at x by

$$R_x^M(u, v)w := \nabla_u \nabla_v w(x) - \nabla_v \nabla_u w(x) - \nabla_{\nabla_u v} w(x) + \nabla_{\nabla_v u} w(x).$$

If in particular u, v are also linearly independent at x , then we define the (tangential) *sectional curvature* $K_x^M(u, v)$ at x along the section $\sigma_M^2 = \text{span}(u, v)$ by

$$K_x^M(u, v) := \frac{\langle R_x^M(u, v)v, u \rangle}{\langle u, u \rangle \langle v, v \rangle - \langle u, v \rangle^2}.$$

4.30 Remark: The sectional curvature can locally be seen as the Gaussian curvature of a surface whose tangent plane is spanned by u and v : Taking two geodesics χ_u, χ_v through a point $y \in M$ with tangent directions $u(y), v(y)$, this local surface is obtained as the image of the plane spanned by the preimages of these geodesics under the exponential map⁽⁹⁾ for y , so $\exp_{y,M}(uu + vv)$ for $u, v \in]-\varepsilon, \varepsilon[$.

We now give two useful properties for the curvature tensor from [51, Prop. 3.5]:

4.31 Lemma Let $y \in M$ and let $u, v, w, x \in \Gamma(M)$ such that u and v are linearly independent near y . Then the curvature tensor satisfies locally around y the relations

$$R_y^M(u, v)x = -R_y^M(v, u)x, \quad \langle R_y^M(u, v)w, x \rangle = -\langle R_y^M(u, v)x, w \rangle.$$

⁽⁹⁾Cf. Sect. 9.1.1 for definition and properties of the exponential map.

Moreover, $R_y^M(u, v)x$ vanishes at y whenever the vector field x is parallel on M . Consequently, the curvature tensor vanishes identically for such parallel x .

Proof: The first two properties are proven in [51, Prop. 3.5], and the first one is also fairly obvious. The claim on parallel fields follows then by insertion. \square

Now we can finally deduce the desired relation for the kernel of the tangential Hessian. It turns out to be a direct consequence of the following lemma:

4.32 Lemma *Let $M \in \mathbb{M}_{\text{sd}}^k(\mathbb{R}^d)$ and let $f \in C^2(M)$ be a nonconstant function such that its tangential Hessian vanishes identically. Let $u \in \Gamma(M)$ be a vector field that is linearly independent to the gradient field at $x \in M$. Then the sectional curvature $K_x^M(\nabla_M f, u)$ vanishes at x .*

Proof: As the tangential gradient $\nabla_M f$ must have constant norm over all of M , we know that $\nabla_M f$ does not vanish anywhere. Hence it is a smooth, nonvanishing integrable vector field on M that is parallel as well. But by Lemma 4.31, the curvature tensor $R_x^M(u, v)\nabla_M f$ must vanish identically at any $x \in M$ for any vector fields $u, v \in \Gamma(M)$ that are linearly independent near x . This gives in particular that the sectional curvature must vanish at any x for any section that contains $\nabla_M f$. \square

This last result is now the direct justification of the following condition:

4.33 Theorem *If $M \in \mathbb{M}_{\text{sd}}^k(\mathbb{R}^d)$ contains a point ξ such that for any two vector fields $u, v \in \Gamma(M)$ that are linearly independent at ξ the sectional curvature does not vanish at ξ , then the tangential Hessian vanishes only for constant functions and any nonempty $\Xi \subseteq M$ is D_M^2 -unisolvent.*

If in particular $k = 2$ and the Gaussian curvature of M does not vanish identically, then any nonempty $\Xi \subseteq M$ is D_M^2 -unisolvent.

Proof: The general statement is obvious by the previous lemmas, and the particular statement for surfaces comes because for a surface, there is only one sectional curvature, as any section coincides with the whole tangent bundle. And that sectional curvature coincides with the Gaussian curvature of that surface (cf. [73, pp. 145/146]). \square

4.2.2 Unisolvency and Isometry

The last theorem implies that in the surface case, nonconstant functions can have identically vanishing Hessian only if the Gaussian curvature of the surface vanishes identically, too. Surfaces whose Gaussian curvature vanishes identically are called *developable surfaces*, and they can locally be obtained by "rolling up" a portion of the plane in an isometric way. Following [34, Ch. 1, Def. 2.2], a diffeomorphism

$\varphi : \omega \rightarrow M$ with $\omega \subseteq \mathbb{R}^k$ and $\varphi(\omega) \subseteq M$ is called an *isometry* between ω and $\varphi(\omega)$ if for any $v, w \in \mathbb{R}^k$ and any $x \in \omega$ it holds

$$\langle v, w \rangle = \langle D\varphi(x)v, D\varphi(x)w \rangle.$$

Correspondingly, a local diffeomorphism is called a *local isometry* if the respective relation holds locally.

4.34 Remark: This implies in particular that the linear map $D\varphi(x) : \mathbb{R}^k \rightarrow T_{\varphi(x)}M$ is an orthogonal linear map.

We deduce now that if a function $f : M \rightarrow \mathbb{R}$ for $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ has identically vanishing Hessian and $\varphi : \omega \rightarrow M$ is an isometry, then $f \circ \varphi$ must be a linear polynomial on ω . This becomes apparent if we consider the following lemma. It states a relation in terms of tangential differential calculus that is one of the key relations of Riemannian geometry in the general case.

4.35 Lemma *Let $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ and let $\varphi : \omega \rightarrow M$ be a smooth isometry between $\omega \subseteq \mathbb{R}^k$ and $\varphi(\omega) \subseteq M$. Then φ preserves tangential derivatives and covariant derivatives. In particular, it preserves parallelism.*

Proof: First we consider an arbitrary smooth function $g : M \rightarrow \mathbb{R}$. By the chain rule it is clear that

$$D(g \circ \varphi)(x) = Dg(\varphi(x)) \cdot D\varphi(x),$$

and by definition, $D\varphi(x)$ maps vectors in \mathbb{R}^k into the tangent space $T_{\varphi(x)}M$ for any $x \in \omega$. As $D\varphi$ is an orthogonal linear map, it gives us a locally smooth orthonormal frame of the tangent space. Then the very definition of tangential derivatives implies

$$D(g \circ \varphi)(x) = D_M g(\varphi(x)).$$

Because the tangential covariant derivative is defined by component-wise application of tangential differentiation, the remaining claims are direct consequences of this relation. \square

However, vanishing Gaussian curvature is only a necessary condition, not a sufficient one. Still, any value of $\ell \in \{0, 1, 2\}$ for the number of basis fields can and does actually occur:

$\ell = 2$ is obviously represented by a domain in \mathbb{R}^2 , and by the last lemma this is retained if we deform that domain isometrically. The case $\ell = 1$ is represented by a cylinder and the case $\ell = 0$ is represented by a truncated cone or a flat torus (with or without holes); to see this, we could use the techniques we already have

at hand at this point, but the necessary arguments would be very specific to the respective situations. So instead of doing that, we will present a more general characterisation of unisolvency in terms of (Riemannian) developing and covering maps. These two extraordinary types of locally isometric maps from and to an ESM are introduced in the following definition.

4.36 Definition Let $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ and let $\omega \in \text{Lip}_k^*$ be connected.

1. A smooth, surjective map $\varphi : \omega \rightarrow M$ is called a *covering (map)*⁽¹⁰⁾ of M if for any $x \in M$ there is a neighbourhood $\Theta(x) \subseteq M$ such that

$$\varphi^{-1}(\Theta(x)) = \bigcup_{j \in J(x)} \Theta_j^\omega(x),$$

where the sets $\{\Theta_j^\omega(x)\}$ are disjoint open subsets of ω such that $\varphi|_{\Theta_j^\omega(x)} : \Theta_j^\omega(x) \rightarrow \Theta(x)$ is a diffeomorphism. It is called a *Riemannian covering (map)* of M if each $\varphi|_{\Theta_j^\omega(x)} : \Theta_j^\omega(x) \rightarrow \Theta(x)$ is an isometry.

2. A smooth map $\pi : M \rightarrow \mathbb{R}^k$ is called a (global) *developing (map)* of M if for any $x \in M$ there is a neighbourhood $\Theta(x) \subseteq M$ of x such that $\pi|_{\Theta(x)}$ is a diffeomorphism of $\Theta(x)$ onto $\pi(\Theta(x))$. It is further called a (global) *Riemannian developing (map)* of M if each $\pi|_{\Theta(x)}$ is an isometry.

If we have a Riemannian covering or developing map, then we can deduce necessary and sufficient condition for unisolvency. We start with the case of a Riemannian developing:

4.37 Theorem Let $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ admit a Riemannian developing $\pi : M \rightarrow \mathbb{R}^k$ and let $\Xi \subseteq M$ be finite. Then the set Ξ is D_M^2 -unisolvent if and only if the set $\pi(\Xi) \subseteq \mathbb{R}^k$ is $P^2(\mathbb{R}^k)$ -unisolvent.

If in the same setting Ξ is not unisolvent, then in particular $\pi(\Xi)$ is part of an affine subspace $V_0 + \gamma_0$ of \mathbb{R}^k . The normal space V_0^\perp to this subspace determines the integrable, nonvanishing parallel gradient fields of any function that vanishes in Ξ in the following way: Any such gradient field has the form

$$(D\pi(x))^t \nu$$

for a constant nonvanishing vector $\nu \in V_0^\perp$ and any maximal system of linearly independent gradient fields of that form has $\dim(V_0^\perp)$ elements.

Proof: Let f be a smooth function whose tangential Hessian vanishes identically on M . Then the function $f \circ \pi^{-1}$ has to be a linear polynomial on any domain $\pi(\Theta(x))$: By Lemma 4.35 we can deduce that in particular tangential and covariant

⁽¹⁰⁾The letter "Q, q" is the greek letter "Koppa/Qoppa" representing the latin "Q". It fell out of use in attic greek during the classical era, remaining only as a numeral sign.

derivatives are preserved locally by local isometries, and these reduce to standard derivatives in any $\pi(\Theta(x))$; so the standard (Euclidean) Hessian of $f \circ \pi^{-1}$ must vanish there and thus $f \circ \pi^{-1}$ is a linear polynomial on any such set $\pi(\Theta(x))$. Now we notice that on any two $\pi(\Theta(y)), \pi(\Theta(z))$ with nonempty intersection these polynomials have to coincide. Consequently, they have to coincide globally and we can thus conclude directly on sufficiency.

To prove necessity, we provide a suitable integrable parallel vector field if the stated requirement is violated. If the points of $\pi(\Xi)$ are not $P^2(\mathbb{R}^k)$ -unisolvent, then by [105] they lie in an affine subspace $V_0 + \gamma_0$ of \mathbb{R}^k . So we can choose at least one fixed unit normal to this subspace, say $\nu^1 \in \mathbb{S}^{k-1}$. Then we define a function $p_1(z) := z^t \nu^1$ for $z \in \omega$, which is a linear polynomial in ω . If we now define $f_1(x) := p_1(\pi(x))$, then as isometries preserve the tangential and covariant derivative, f_1 must have vanishing Hessian. Repeating this process for further mutually orthogonal vectors $\nu^2, \dots, \nu^\ell \in \mathbb{S}^{k-1}$ from the normal space V_0^\perp determines a set of functions that are obviously linearly independent, and the set of corresponding fields is maximal by construction. \square

The important advantage of this characterisation is that we do not need a global isometry, a local but surjective isometry is sufficient. This can provide considerable advantage, as Fig. 4.1 shows: On the one hand, the surface depicted there from above and from behind is not globally isometric to any domain in \mathbb{R}^2 . On the other hand, as it has curvature only in one direction like a cylinder, it is easily mapped into a domain in the Euclidean plane globally such that the map is locally isometric. Thus it suffices to consider the image of Ξ under this map to deduce unisolvency.

Unfortunately, we cannot apply the same idea directly if instead of a developing we have a covering of M . In that case, we would have to insert φ^{-1} into the linear

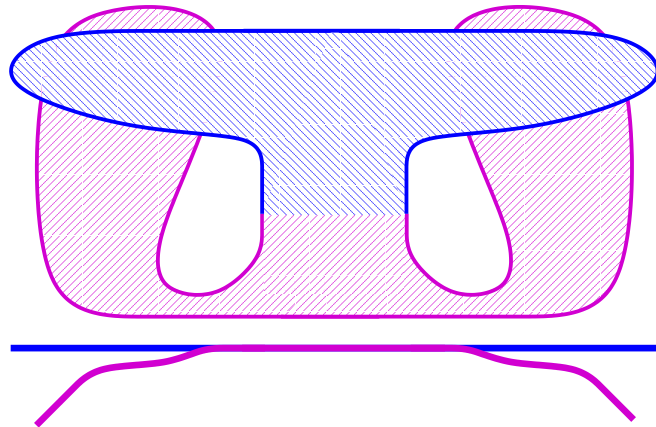


Figure 4.1: Is a surface with vanishing Gaussian curvature, locally isometric to \mathbb{R}^2 from above (upper graphic) and from behind (lower graphic). The respective blue and purple parts are isometric to \mathbb{R}^2 .

polynomial, which is not necessarily well-defined. But actually, this already gives us a hint what to do: All polynomials where $p \circ \varphi^{-1}$ is not well-defined turn out to be invalid choices.

4.38 Lemma *Let $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ and let $\omega \subseteq \mathbb{R}^k$ be path-connected. Let $\varphi : \omega \rightarrow M$ be a Riemannian covering of M . Then a nonconstant function $f \in C^2(M)$ has identically vanishing tangential Hessian if and only if there is a polynomial $p \in P^2(\mathbb{R}^k)$ such that locally $p = f \circ \varphi$ and*

$$p(x) = p(y) \text{ for any } x, y \in \varphi^{-1}(\{z\}) \text{ and arbitrary } z \in M.$$

Proof: This becomes clear by arguments very similar to those provided to prove the conditions in case of a developing map: To see sufficiency, we notice again by Lemma 4.35 that $f \circ \varphi$ is a linear polynomial on any $\Theta_j^\omega(x) \subseteq \omega$. On any two such $\Theta^\omega(y), \Theta^\omega(z)$ with nonempty intersection these polynomials have to coincide. Consequently, $f \circ \varphi$ is globally a polynomial as well, which gives sufficiency. For necessity, we see that by the same arguments, we *must* be able to deduce a polynomial that coincides with $f \circ \varphi$ locally, and by connectivity this polynomial must be valid globally. \square

With this lemma, the next theorem is effectively already proven and gives us finally a characterisation of unisolvent sets also for the case of a covering of M .

4.39 Theorem *Let $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$, let $\Xi \subseteq M$ be finite and let $\omega \subseteq \mathbb{R}^k$ be path-connected. Let $\varphi : \omega \rightarrow M$ be a Riemannian covering map of M . Let $V_0 \subseteq \mathbb{R}^k$ be the vector subspace spanned by*

$$\{x - y : x, y \in \omega, x \neq y, \varphi(x) = \varphi(y)\}.$$

Let V_0^\perp be its orthogonal complement. Then Ξ is D_M^2 -unisolvent if and only if the set $\Pi_{V_0^\perp} \varphi^{-1}(\Xi)$ is unisolvent for the space $P^2(V_0^\perp)$.

Proof: With the last lemma, there is not much left to do: As $f \circ \varphi$ must be a well-defined linear polynomial, and must have the same function value in any two $x, y \in \varphi^{-1}(\{z\})$ for an arbitrary $z \in M$, it must be constant on the line that joins them. Thus this line is part of a level set. Consequently, the gradient of $f \circ \varphi$ must be orthogonal to any of these lines, and so to the whole subspace they span. This reduces the available degrees of freedom from $P^2(\mathbb{R}^k)$ to $P^2(V_0^\perp)$. As on the other hand any polynomial in $P^2(V_0^\perp)$ can then be used to obtain a function with identically vanishing tangential Hessian, we obtain the claimed relation. \square

We now revise the examples we have mentioned before: Generalised cylinder, gen-

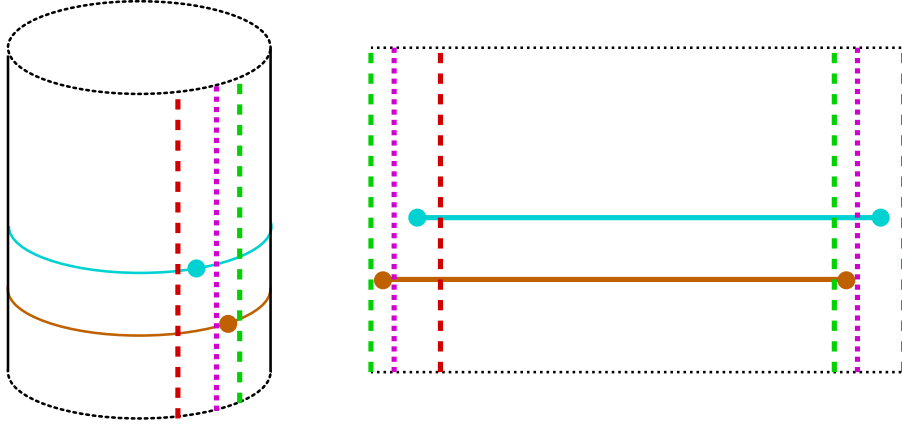


Figure 4.2: Cylinder surface in space and “unrolled” cylinder, with overlapping area bounded by dashed red and green lines. The teal and brown points have two preimages, and the lines that link them specify the direction to which the gradient of the polynomial must be normal.

eralised cone and flat torus. First we consider a generalised cylinder, that is a cartesian product of a smoothly closed curve $\gamma \subseteq \mathbb{R}^2$ and an open interval I . A local isometry that maps this cylinder into the Euclidean plane is fairly obvious, as depicted in Fig. 4.2: One simply has to “unroll” the cylinder into the plane. In the figure, we find this presented exemplarily for a circular cylinder, but other curves can be handled in the same way.

We obtain the covering map by the inverse of this, so rolling up the cylinder again. As all lines that link two points assigned to the same point on the cylinder have the same direction, we retain one free parameter for the gradient: The direction orthogonal to the “rolling direction”. This remains valid if we carve out holes in the cylinder, as long as there are still points on the cylinder that have two preimages within the same connected component of the “unrolling”.

4.40 Remark: We can also express this unrolling as the action of a translation by a fixed value in a specific direction (the period and direction of the “unrolling”), and consider all points on the cylinder as equivalence classes in \mathbb{R}^2 under this translation. In that sense, the free parameter is the direction in which points are not affected by the translation. More generally speaking, we can choose only those directions that are orthogonal to the orbits of the action “translation by fixed value $(a, b) \neq (0, 0)$ ”.

Very similar to the cylinders are the flat tori. With the Clifford torus, we have already encountered a flat torus in the examples for ambient spline approximation. We recall here that it is obtained as the surface

$$\mathbb{T}_{\text{clf}} = \left(\frac{1}{\sqrt{2}} \mathbb{S}^1 \right) \times \left(\frac{1}{\sqrt{2}} \mathbb{S}^1 \right),$$

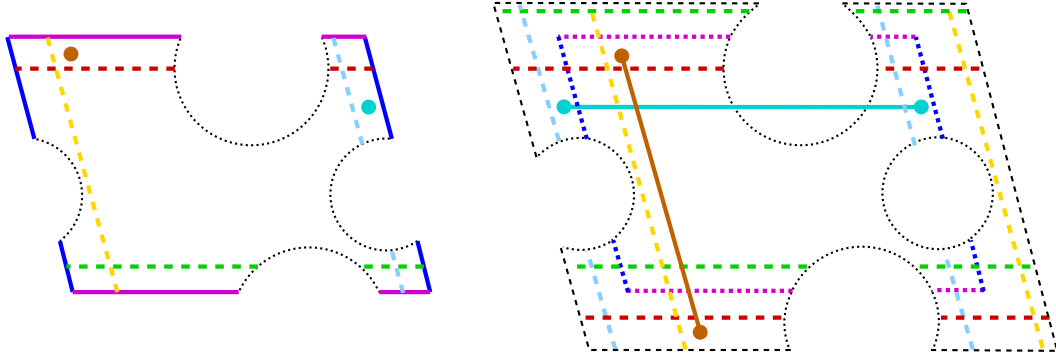


Figure 4.3: Flat torus with holes and a suitable set ω for a Riemannian covering, with overlapping area bounded by dashed red and green or by the blue and yellow lines, respectively. The teal and brown points have two preimages, and the lines that link them specify the direction to which the gradient of the polynomial must be normal.

and can be mapped into the square $[0, \pi\sqrt{2}] \times [0, \pi\sqrt{2}]$ isometrically with identification of opposite edges. In the same way, other flat tori can be obtained by other squares or more generally even by identification of opposite edges in a parallelogram.

Again, it is easy to find a suitable covering that is locally an isometry: We just have to copy the parallelogram several times, translate it suitably and “glue” it to the original parallelogram on each edge and on each corner. As depicted in Fig. 4.3, a subset of the resulting set that contains the relative closure of the original parallelogram is then a valid choice for ω .

If we do not extinguish an entire identified edge, then there will be two linearly independent directions that are ruled out by the lines that link points with multiple preimages: Both edge directions of the parallelogram do that. Consequently, any nonempty set is D_M^2 -unisolvent in that case. And if we extinguish an entire identified edge, we effectively end up with a cylinder we have already dealt with.

4.41 Remark: As in the case of cylinders, the tori can be seen as equivalence classes under translations; just there are two linearly independent translations this time. As there are, consequently, also two linearly independent orbits, we see also from this point of view that there is no suitable gradient direction remaining.

Finally, we turn to a truncated generalised cone, so a surface obtained from a closed curve $\gamma \subseteq \mathbb{R}^2$ that is arc-length parameterised in the form $\gamma : [0, L[\rightarrow \gamma$ and a point $(x_0, y_0, z_0)^t$ with $z_0 \neq 0$ in the form

$$\{\eta(x_0, y_0, z_0)^t + (1 - \eta)(\gamma_1(t), \gamma_2(t), 0)^t : \eta \in]\eta_1(t), \eta_2(t)[, t \in [0, L]\},$$

where $\eta_1, \eta_2 : [0, L] \rightarrow]0, \infty[$ are smooth bounded functions such that in particular $\eta_1(t) < \eta_2(t)$ for all $t \in [0, L]$.

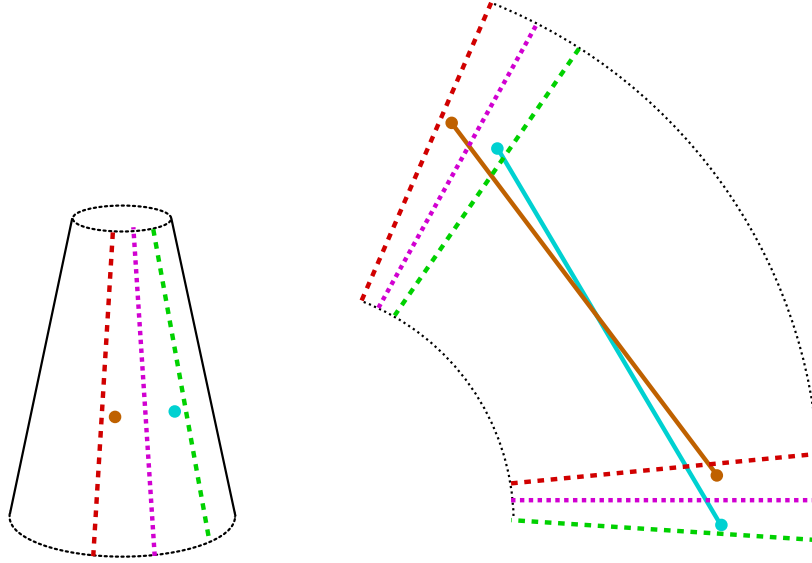


Figure 4.4: Truncated cone and a suitable set ω for a Riemannian covering, with overlapping area bounded by dashed red and green lines, respectively. The teal and brown points have two preimages, and the lines that link them specify the direction to which the gradient of the polynomial must be normal.

For this kind of developable surface, the unrolling appears in a different way: One lays the (not yet truncated) cone on the plane, fixes the apex of the cone, and unrolls “around” the apex — which remains valid if just a subsurface is considered. If we arrive at the same line segment on the cone through the apex that touched the plane in the beginning before we have passed a full rotation by $2\pi^{(11)}$, then identification of these edges and slightly extending before and after will give us the covering we need. We see the respective relation in Fig. 4.4. There we see also two points with two preimages that will have linearly independent distance vectors, so again we see that there is no suitable gradient direction remaining.

4.42 Remark: In contrast to cylinders and tori, the cone can be considered as equivalence classes under rotations, not translations. If these rotations are based on angles that are no multiples of 2π , then it is directly clear that the links between two orbits yield two linearly independent directions. However, if the rotation angle is indeed 2π , then the cone is flat, so it has actually no height and is a mere subset of the unit ball of \mathbb{R}^2 — and then it is clear by standard arguments that we need three points that do not lie on the same line.

4.43 Remark: One important point in these examples is that they effectively characterise all developable surfaces in \mathbb{R}^3 already: As stated in [71, Th. 3.7.1], all developable surfaces in \mathbb{R}^3 are locally either a generalised cone, a generalised cylinder or a so-called *tangent developable*, which is known to be *globally* isomet-

⁽¹¹⁾This will never happen if the curve is a circle, for instance.

ric to a subdomain of \mathbb{R}^2 (cf. [69, Th. 55.2/55.3] or [71, Th. 3.7.1]). Thus we have effectively characterised the totality of developable surfaces in \mathbb{R}^3 with respect to unisolvency.

In that respect, one should particularly bear in mind that if there are only ℓ parallel fields on a subsurface of a surface, then there are no more than ℓ parallel fields on the whole surface as well. So whenever a subsurface is a generalised cone that is not isometric to a subsurface of the plane, or a generalised cylinder with the same property, then there are no or at most one parallel fields, respectively.

4.3 Tangential Bilinear Functionals and Tangential Energies

Now that we have defined suitable conditions for points to fix the kernel of $\mathcal{E}_H(f, f)$, we will turn to defining an energy functional thereby. Our primary goal will be to achieve that the square root of $\mathcal{E}_H^\Xi(f, f)$ for

$$\mathcal{E}_H^\Xi(f, g) = \mathcal{E}_H(f, g) + \sum_{\xi \in \Xi} f(\xi) \cdot g(\xi)$$

yields an equivalent norm on $H^2(\mathcal{M})$ whenever Ξ is unisolvent. If we then fix the function values, we are in a position to generalise the energy minimisation problem solved by cubic splines in the univariate case to our setting of ESMs. But in the course of this, we will find that there are numerous other reasonable energy functionals one can employ; some of these have a similar meaning to the one presented above, while others can be used to characterise the solutions of certain elliptic partial differential equations. We begin with a rather general treatment of functionals on $H^2(\mathcal{M})$, and deduce $\mathcal{E}_H^\Xi(f, f)$ as well as specific other functionals as special cases in the aftermath.

Crucial to our theory is the following definition. It introduces a number of important properties according to [16, 37, 52, 107] for an arbitrary generic Hilbert space H . We will specifically choose $H = H^2(\mathcal{M})$ later.

4.44 Definition A symmetric bilinear functional $B : H \times H \rightarrow \mathbb{R}$ on some Hilbert space H is called a *continuous functional* if there is a constant $c_1 > 0$ such that

$$B(f_1, f_2) \leq c_1 \|f_1\|_H \|f_2\|_H$$

for any $f_1, f_2 \in H$. It is called *elliptic* if there is a constant $c_2 > 0$ such that for any $f \in H$

$$\|f\|_H^2 \leq c_2 B(f, f).$$

Moreover, it is called *strictly convex* if for any two unequal $f, g \in H$ and $\lambda \in]0, 1[$

$$B(\lambda f + (1 - \lambda)g, \lambda f + (1 - \lambda)g) < \lambda B(f, f) + (1 - \lambda)B(g, g).$$

A functional $F : H \rightarrow \mathbb{R}$ is called *coercive* if

$$\|f\|_H^2 \rightarrow \infty \implies F(f) \rightarrow \infty.$$

4.45 Important: We point out that from here on we demand that any bilinear form is symmetric. We further declare here that we omit the second functional argument when they coincide, so $B(g) = B(g, g)$, for the sake of brevity in notation.

4.46 Remark: (1) In a Hilbert space, any norm is necessarily convex. So for any two $f \neq g$ with norm 1 and $\lambda \in]0, 1[$ it holds

$$\|\lambda f + (1 - \lambda)g\| < \lambda \|f\| + (1 - \lambda) \|g\|.$$

(2) In the course of this thesis, we will only consider functionals F of the form $F(f) = B(f) + \Lambda(f)$ for a quadratic $B(f)$ derived from bilinear form $B(f, g)$ and a linear functional Λ . As these are effectively determining an energy on $H^2(M)$, we will write \mathcal{E} instead of F . If then in particular $\mathcal{E}(f) = B(f) + \Lambda(f)$ for an elliptic bilinear functional B , then \mathcal{E} is obviously coercive.

Once we have chosen a functional that is continuous, coercive and convex, it is not hard to see that it attains its minimum on any convex closed subset of the Hilbert space. In particular, any Hilbert space norm has a minimum in such subset (cf. [16, Cor. 3.23]). The latter is clear to be zero for the whole space, but more interesting for convex subsets. We sum this up in a proposition:

4.47 Proposition *Let F be a convex, continuous and coercive functional on a closed, convex subset D_{co} of Hilbert space H . Then there is an element $f^* \in D_{\text{co}}$ such that for any $f \in D_{\text{co}}$ the relation $F(f^*) \leq F(f)$ holds, so F attains its minimum.*

4.48 Remark: Note that the above result states no requirements on strict convexity, but also makes no statement on uniqueness. However, the minimum is clearly unique if the functional is strictly convex.

Most important for us will be the fact that those functions in $H^2(M)$ which coincide on a finite set of points Ξ form a closed convex subset of that space, provided point evaluation is continuous there: Convexity comes directly by the interpolation constraints, and closedness is a consequence of the well-known fact that preimages of closed sets under continuous mappings are closed.

4.3.1 Some Specific Energy Functionals

After these introductory statements, we can now become more concrete: We will see now that the energy functional \mathcal{E}_H^Ξ is elliptic on $H^2(\mathcal{M})$ and so its square root gives us an equivalent norm. And afterwards, we deduce corresponding results for a couple of other functionals that turn out to be continuous and coercive w.r.t. the $H^2(\mathcal{M})$ -norm.

4.49 Theorem *For any $\mathcal{M} \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ of dimension $k \leq 3$ and any fixed $D_{\mathcal{M}}^2$ -unisolvent set Ξ , the functional $\mathcal{E}_H^\Xi(f, g)$ is continuous and elliptic.*

Proof: The first inequality $\mathcal{E}_H^\Xi(f, g) \leq c \|f\|_{H^2} \|g\|_{H^2}$ is fairly obvious, since by the Sobolev embedding theorem stated in the appendix, we have $H^2(\mathcal{M}) \hookrightarrow C(\mathcal{M})$, and so point evaluations are continuous in $H^2(\mathcal{M})$ and therefore bounded. So we have to work only for the other inequality and hence have to prove ellipticity of \mathcal{E}_H^Ξ . This is done along the steps proposed in the proof of [105, Lem. 11.35] for the Euclidean case: By Rellich-Kondrachov's Embedding Theorem 9.10 the embedding $H^2(\mathcal{M}) \hookrightarrow H^1(\mathcal{M})$ is compact in our case. Assume now that there were a sequence $(g_n)_{n \in \mathbb{N}}$ in $H^2(\mathcal{M})$ such that $\|g_n\|_{H_T^2(\mathcal{M})}^2 = 1$ for all n and nonetheless

$$\sum_{\xi \in \Xi} |g_n(\xi)|^2 + \mathcal{E}_H(g_n) < \frac{1}{n}.$$

This gives in particular that $\mathcal{E}_H^\Xi(g_n)$ approaches zero for $n \rightarrow \infty$. By the compact embedding stated above, $(g_n)_{n \in \mathbb{N}}$ must have a convergent subsequence, say (\tilde{g}_n) with limit $\tilde{g} \in H^1(\mathcal{M})$. On the other hand, since

$$\mathcal{E}_H(\tilde{g}_n) \rightarrow 0,$$

(\tilde{g}_n) is Cauchy in $H^2(\mathcal{M})$ for the equivalent norm $\|\cdot\|_{H_T^2}$. Therefore it must have a limit there, and by uniqueness this limit must coincide with \tilde{g} , and we must have $\mathcal{E}_H(\tilde{g}, \tilde{g}) = 0$. Moreover we have by definition of $(g_n)_{n \in \mathbb{N}}$ that $\tilde{g}_n(\xi) \rightarrow 0$ for any $\xi \in \Xi$. As the Sobolev embedding theorem guarantees continuity of any function in $H^2(\mathcal{M})$ we get $\tilde{g}_n(\xi) \rightarrow \tilde{g}(\xi)$ and thus $\tilde{g}(\xi) = 0$. Due to our condition on Ξ we can only have $\tilde{g} = 0$ satisfying this condition. But then we have a contradiction, as we assumed $\|\tilde{g}_n\|_{H_T^2(\mathcal{M})}^2 = 1$. \square

4.50 Corollary *For any $D_{\mathcal{M}}^2$ -unisolvent set Ξ and corresponding function values Y_Ξ , the functional $\mathcal{E}_H(f)$ is strictly convex, continuous and elliptic on the set*

$$\{f \in H^2(\mathcal{M}) : f(\xi) = \gamma_\xi, \xi \in \Xi, \gamma_\xi \in Y_\Xi\}.$$

There are numerous other functionals and corresponding norms one can define. In this chapter, we will just consider a couple of further prominent and important examples, all of them either based on the Hessian or the Laplace-Beltrami operator. To analyse the latter, we need an appropriate version of the *Calderon-Zygmund inequality* on compact ESMs that can be found in [57, Sect. 4] for the $H^2(\mathbb{M})$ -dense subset of compactly supported smooth functions (cf. [63]) and thus generalises directly:

4.51 Proposition — Calderon-Zygmund Inequality —

Let $\mathbb{M} \in \mathbb{M}_{\text{cp}}^k(\mathbb{R}^d)$. Then for some $c_1, c_2 > 0$ and any $f \in H^2(\mathbb{M})$ we have

$$\sqrt{\epsilon_{\mathbb{H}}(f, f)} \leq c_1 \|f\|_{L_2(\mathbb{M})} + c_2 \|\Delta_{\mathbb{M}} f\|_{L_2(\mathbb{M})}.$$

With this result it is not hard to deduce the following result for compact ESMs, which allows us to consider Laplace-Beltrami instead of the Hessian:

4.52 Corollary For any ESM $\mathbb{M} \in \mathbb{M}_{\text{cp}}^k(\mathbb{R}^d)$ of dimension $k \leq 3$ and any nonempty set Ξ , the Laplacian energy functional $\epsilon_{\Delta}^{\Xi}(f, g) := \epsilon_{\Delta}(f, g) + \sum_{\xi \in \Xi} f(\xi) \cdot g(\xi)$ for

$$\epsilon_{\Delta}(f, g) := \int_{\mathbb{M}} \epsilon_{\Delta}(f, g) \text{ with } \epsilon_{\Delta}(f, g) = (\Delta_{\mathbb{M}} f)(\Delta_{\mathbb{M}} g)$$

is continuous and elliptic.

Proof: We can bound $\epsilon_{\Delta}^{\Xi}(f, g) \leq c \epsilon_{\mathbb{H}}^{\Xi}(f, g) \leq c \|f\|_{H^2(\mathbb{M})} \|g\|_{H^2(\mathbb{M})}$, so continuity comes directly once more, and only the other relation is of interest again. But now we have Calderon-Zygmund, and thereby we obtain

$$\|f\|_{H^2_{\mathbb{T}}(\mathbb{M})}^2 \leq c \left(\|f\|_{H^1_{\mathbb{T}}(\mathbb{M})}^2 + \|\Delta_{\mathbb{M}} f\|_{L_2(\mathbb{M})}^2 \right) =: \|f\|_{H^2_{\Delta}(\mathbb{M})}^2$$

by adding $\|f\|_{H^1_{\mathbb{T}}(\mathbb{M})}^2$ on both sides. This gives equivalence⁽¹²⁾ of $\|\cdot\|_{H^2(\mathbb{M})}$ and the auxiliary norm $\|\cdot\|_{H^2_{\Delta}(\mathbb{M})}$. Consequently, we can more or less copy the proof of Theorem 4.49; we just have to replace the tangential Hessian energy by the Laplacian energy if we recall that in compact ESMs a single point suffices to force a function with vanishing Laplace-Beltrami to vanish if interpolating zero. \square

From these functionals, one can easily deduce others and obtain continuity, strict convexity and coercivity or even ellipticity for them. In particular, we have the respective result for the functional

$$\epsilon_{\eta}^{\Xi}(f) := \eta \cdot \epsilon_{\mathbb{H}}(f) + (1 - \eta) \cdot \sum_{\xi \in \Xi} (f(\xi) - \gamma_{\xi})^2$$

⁽¹²⁾In fact, one can also find in [36, Lem. 3.2] that the standard norm on $H^2(\mathbb{M})$ and this auxiliary norm are equivalent, at least for the hypersurface case.

for D_M^2 -unisolvent Ξ , $\eta \in]0, 1[$ and arbitrary $(\gamma_\xi)_{\xi \in \Xi}$ on $H^2(M)$, provided we have $\dim M = k < 4$: We see continuity directly from our previous arguments and the fact that by Sobolev embedding point evaluation is continuous on $H^2(M)$ if $\dim M < 4$; in fact, $\mathcal{E}_\eta^\Xi(f)$ differs from $\mathcal{E}_H^\Xi(f)$ only by scalar multiplication and the affine linear term

$$\eta \cdot \sum_{\xi \in \Xi} \left((\gamma_\xi)^2 - 2f(\xi)\gamma_\xi \right),$$

which is easily seen to be continuous. Strict convexity is clear by the corresponding property of $\mathcal{E}_H^\Xi(f)$, as an additional constant or linear portion will not affect this, and coercivity comes by the ellipticity of $\mathcal{E}_H^\Xi(f)$.

4.53 Remark: We can actually be more general in this setting: We can replace η by a $C^\infty(M)$ -function $\eta : M \rightarrow [a, b]$ with $0 < a < b < \infty$ and $(1 - \eta)$ by pointwise weights $\mathcal{H}_\Xi = \{\eta_\xi\}^{(13)}$ with $0 < \eta_\xi < \infty$ for each $\xi \in \Xi$ without doing any harm to the relevant properties. These choices yield different levels of detail for a smoothing or balancing process on $H^2(M)$. That process is then capable of stressing smoothness in terms of Hessian energy or approximation in a finite set of points both globally and locally, similar to the usual formulation of smoothing splines (cf. [33]). And in the course of this thesis, we will revisit this and the previous functionals to achieve indeed corresponding approximations of energy minima under point constraints and smoothing!

After discussing functionals based on certain energy norms accompanied by point evaluations up to this point, we now turn to another useful functional where there are no point evaluations, but which provides nonetheless all relevant properties. This is a functional that will allow us later to solve the partial differential equation $\Delta_M f - \lambda f = g$ on a compact ESM without boundary, provided this solution exists and is an element of $H^2(M)$:

4.54 Theorem *The functional*

$$\mathcal{E}_\Delta^\lambda(f) := \int_M (\Delta_M f - \lambda f)^2$$

is continuous and elliptic on $H^2(M)$ for any $M \in \mathbb{M}_{\text{cp}}^k(\mathbb{R}^d)$ and any $\lambda > 0$.

Proof: We obtain by Green's theorem that

⁽¹³⁾The letters \mathcal{H}, \mathcal{h} are a variant of the greek letter "Digamma/Wau", representing the sound "[w]" of standard English like in "weight". We use this here because apparently a sound with value "[w]" is the first hand choice for such set of weights, and both standard latin "W" and standard greek "Digamma"-glyph "F" would obviously be misleading. Additionally, \mathcal{H}/\mathcal{h} is also the cyrillic successor of greek "H, η", making \mathcal{H} also the closest relative to uppercase η from a certain point of view.

$$\begin{aligned} \int_{\mathbb{M}} (\Delta_{\mathbb{M}} f - \lambda f)^2 &= \int_{\mathbb{M}} (\Delta_{\mathbb{M}} f)^2 - 2\lambda \int_{\mathbb{M}} f \Delta_{\mathbb{M}} f + \lambda^2 \int_{\mathbb{M}} f^2 \\ &= \int_{\mathbb{M}} (\Delta_{\mathbb{M}} f)^2 + \lambda^2 \int_{\mathbb{M}} f^2 + 2\lambda \int_{\mathbb{M}} \langle \nabla_{\mathbb{M}} f, \nabla_{\mathbb{M}} f \rangle \end{aligned}$$

which is up to weighting factors λ, λ^2 precisely the auxiliary norm $\|f\|_{H_{\Delta}^2(\mathbb{M})}^2$. \square

As a result of this, we see that $\sqrt{\mathbb{E}_{\Delta}^{\lambda}(\cdot)}$ gives us an equivalent norm on $H^2(\mathbb{M})$. If we now demand that there is indeed a solution $f^* \in H^2(\mathbb{M})$ to the partial differential equation $\Delta_{\mathbb{M}} f - \lambda f = g$, then by definition this function satisfies $\Delta_{\mathbb{M}} f^* - \lambda f^* = g$ in the H^2 -sense. Thus we can deduce for any $f \in H^2$ the relation

$$\begin{aligned} \|f - f^*\|_{H^2(\mathbb{M})}^2 &\leq c \mathbb{E}_{\Delta}^{\lambda}(f - f^*) = c \int_{\mathbb{M}} (\Delta_{\mathbb{M}}(f - f^*) - \lambda(f - f^*))^2 \\ &= c \int_{\mathbb{M}} (\Delta_{\mathbb{M}} f - \lambda f - (\Delta_{\mathbb{M}} f^* - \lambda f^*))^2 = c \int_{\mathbb{M}} (\Delta_{\mathbb{M}} f - \lambda f - g)^2, \end{aligned}$$

whereby the residual of the equation is equivalent to the squared norm distance to the solution. Consequently, the solution of the equation reduces to some *residual energy minimisation*.

Similarly, we can also handle the situation $\lambda = 0$, because we already know that for a given function value at a single point ξ_0 (and continuous point evaluation) the energy functional $\mathbb{E}_{\Delta}(f) + (f(\xi_0) - \gamma_0)^2$ is elliptic, and thus for a fixed interpolation constraint $f(\xi_0) = \gamma_0$ and the PDE $\Delta_{\mathbb{M}} f = g$, the residual again turns out to be a squared norm distance to the solution f^* of the form

$$\begin{aligned} \mathbb{E}_{\Delta}(f - g) + (f(\xi_0) - \gamma_0)^2 &= \int_{\mathbb{M}} (\Delta_{\mathbb{M}} f - g)^2 + (f(\xi_0) - \gamma_0)^2 \\ &= \int_{\mathbb{M}} (\Delta_{\mathbb{M}} f - \Delta_{\mathbb{M}} f^*)^2 + (f(\xi_0) - f^*(\xi_0))^2 \\ &\geq c \|f - f^*\|_{H^2(\mathbb{M})}^2. \end{aligned}$$

4.55 Remark: (1) The solvability of even these simple PDEs of the form $\Delta_{\mathbb{M}} f - \lambda f = g$ with $\lambda \geq 0$ is quite a delicate matter, particularly when regularity questions are involved — we recall in particular that we require a solution to be indeed a function from H^2 , while commonly the approach of choice (cf. [37, 52]) are so called *weak solutions*, which can only be expected to be elements of H^1 . However, the general “rule of thumb” for the regularity of a solution is that if $g \in H^{\ell}$ then $f^* \in H^{\ell+2}$ (cf. [37, 52, 55]). Regarding the matter of solvability (which we shall not address any further) at least in case of the equation $\Delta f = g$, an application of Green’s theorem shows that in our case of a compact ESM the function g must necessarily have vanishing integral because it holds

$$\int_{\mathbb{M}} 1 \cdot g = \int_{\mathbb{M}} 1 \cdot \Delta_{\mathbb{M}} f = - \int_{\mathbb{M}} \langle 0, \nabla_{\mathbb{M}} f \rangle = 0.$$

(2) As usual, the presence of a boundary introduces further difficulties. In our case, it would introduce the need for boundary conditions, and we would have to include them in our functionals to maintain ellipticity in the present situation. Indeed, this is possible to some degree (cf. [55]), but unfortunately the inclusion of the boundary conditions into the functional is of fractional Sobolev type and therefore highly uncomfortable in practical terms.

(3) One could also look for an appropriate expression for more general intrinsic partial differential operators and equations (cf. [36, 55]), but the detailed discussion of these would lead too far here. So we leave the transformation of more general intrinsic PDE into our setting to the future.

4.3.2 Functional Residuals and Norm Distances

In some of the previous examples of functionals, differences as arguments lead to equivalent distances in $H^2(\mathbb{M})$. This in mind, we could ask ourselves what we can obtain if we only know about the functional evaluations: Is there a way to deduce $\|f - f^*\|_{H^2(\mathbb{M})}$ from $|\mathcal{E}(f) - \mathcal{E}(f^*)|$ for a functional $\mathcal{E} = B + \Lambda$ with elliptic B , linear Λ and optimum f^* from a convex set $D_{\text{co}} \subseteq H^2(\mathbb{M})$? This is indeed the case, and we can actually deduce a more general result by a simple but elegant trick.

We start for $\mathcal{E} = B + \Lambda$ with continuous linear Λ and continuous bilinear B by defining a smooth function $\varepsilon : [0, 1] \rightarrow \mathbb{R}$ as

$$\varepsilon(t) = \mathcal{E}((1 - t)f^* + tf).$$

If f^* is optimal for \mathcal{E} in D_{co} , this is increasing at $t = 0$. Consequently, the derivative is nonnegative there. We calculate this derivative explicitly now, and we start by inserting $(1 - t)f^* + tf$ into $\mathcal{E} = B + \Lambda$ and applying (bi)-linearity, whereby we obtain

$$\varepsilon(t) = (1 - t)^2 B(f^*) + 2t(1 - t)B(f^*, f) + t^2 B(f) + (1 - t)\Lambda(f^*) + t\Lambda(f).$$

Thereby we can deduce that

$$\varepsilon'(t) = -2(1 - t)B(f^*) + 2(1 - 2t)B(f^*, f) + 2tB(f) - \Lambda(f^*) + \Lambda(f).$$

Thus we obtain that

$$0 \leq \varepsilon'(0) = -2B(f^*) + 2B(f^*, f) + \Lambda(f - f^*).$$

This implies in particular that $-2B(f^*, f) \leq -2B(f^*) + \Lambda(f - f^*)$. Consequently, we can deduce

$$\begin{aligned} B(f - f^*) &= B(f) - 2B(f, f^*) + B(f^*) \leq B(f) - 2B(f^*) + \Lambda(f - f^*) + B(f^*) \\ &= B(f) - B(f^*) + \Lambda(f - f^*). \end{aligned}$$

So we obtain the following important relations, which provide the final statement of these considerations for now:

4.56 Conclusion Let $\mathcal{E} = B + \Lambda$ be a functional with linear Λ and bilinear B and let

$$f^* = \arg \min_{f \in D_{\text{co}}} \mathcal{E}(f).$$

Then it holds for any $f \in D_{\text{co}}$ that

$$B(f - f^*) \leq B(f) - B(f^*) + \Lambda(f - f^*).$$

Consequently, if B is elliptic, then in particular

$$\|f - f^*\|_{H^2(\mathcal{M})}^2 \leq c \cdot B(f - f^*) \leq c |B(f) - B(f^*) + \Lambda(f - f^*)|^2.$$

If furthermore $\Lambda = 0$, then $\|f - f^*\|_{H^2(\mathcal{M})} \leq c |B(f) - B(f^*)|$.

4.4 Approximately Intrinsic Functionals

Now follow some considerations on approximately intrinsic functionals: We will apply finite dimensional function spaces defined on the ambient space in the next chapter, and we cannot really expect the resulting functions to be orthogonal extensions of their restrictions in that situation; for example, this is almost hopeless for TP-splines on an ESM that is not an axis-aligned plane.

On the other hand, our functionals have corresponding formulations in terms of tangent directional Euclidean derivatives of orthogonal extensions. Our hope would be to see that if we insert just some (not necessarily orthogonal) F with $f = T_M F$ in that tangent directional derivative formulation and we can make the normal derivatives approach zero, then⁽¹⁴⁾ we can also approximate the functional value for the function f . Or, more generally speaking, if we have a sequence of functions $(F_n)_{n \in \mathbb{N}}$ such that $T_M F_n = f_n \rightarrow f$ and the normal derivatives of F_n approach zero, do we also obtain that the tangent Euclidean derivative functional values for F_n approach the intrinsic functional value of f ? The answer is indeed affirmative, and

⁽¹⁴⁾as was implied by Theorem 4.7 on the deviations between tangent directional and tangential derivatives

we shall prove this now, beginning with some reconsideration of the functionals we know. Therein, we will see that they all have a common form, leading us to the concept of *equivalently* E_N -extrinsic functionals.

First of all, we recall that any of the specific functionals we have encountered so far has the form

$$\mathcal{E}_M(f) = B_M^0 + B_M^1 + B_M^2 + A_M^\Xi + \Lambda_M,$$

where A_M^Ξ is a possibly empty sum of (weighted) squared function values and each B_M^i is a possibly empty sum of (weighted) integrals taken over squared functionals of i th order tangential differentials. In particular, we have already encountered the choices $B_M^0(f) = \int_M f^2$ and

$$B_M^1(f) = \int_M \langle \nabla_M f, \nabla_M f \rangle$$

$$B_M^2(f) = \int_M \sum_{i,j=1}^k (H_f^M(\tau^i, \tau^j))^2 \quad \text{or} \quad B_M^2(f) = \int_M (\Delta_M f)^2.$$

The only choice for Λ_M we encountered so far was a finite sum of function values in the functional $\mathcal{E}_\eta^\Xi(f)$, so that Λ_M was actually just the linear portion of $A_M^\Xi(f - g_Y)$ for some suitable function g_Y .

By our theory, there is an equivalent way to express these functionals in terms of tangent directional derivatives. We suppose now that $T = (\tau^1, \dots, \tau^k)$ is an orthonormal frame of the pointwise tangent space to M that is locally smooth and C -bounded. Then we have $B_M^1(f) = B_T^1(\vec{F})$ and $B_M^2(f) = B_T^2(\vec{F})$ for $\vec{F} = E_N f$. In our examples, we will therefore choose for the first order functional

$$B_T^1(\vec{F}) = \int_M \sum_{i=1}^d \left(\frac{\partial}{\partial x_i} \vec{F} \right)^2 \quad \text{or} \quad B_T^1(\vec{F}) = \int_M \sum_{i=1}^k (D_{\tau^i} \vec{F})^2.$$

Therein, the latter choice does already present the tangential gradient version: For that choice it holds $B_T^1(F) = B_M^1(f) = B_T^1(\vec{F})$ for *any* smooth F with $f = T_M F$ by definition. For the second order case we will choose B_T^2 in correspondence to the Hessian and Laplacian energies in particular as

$$B_T^2(\vec{F}) = \int_M \sum_{i,j=1}^k (D_{\tau^i} D_{\tau^j} \vec{F})^2 \quad \text{or} \quad B_T^2(\vec{F}) = \int_M (\Delta_T \vec{F})^2.$$

As neither B_M^0 nor A_M^Ξ feature any tangential derivatives, we choose just for the sake of correspondence $B_T^0 = B_M^0$ and $A_T^\Xi = A_M^\Xi$. These observations are the justification to call such functional \mathcal{E}_M in future an *equivalently* E_N -extrinsic functional.

The corresponding expression in terms of tangent directional derivatives is a func-

tional also for more general F with $\mathbb{T}_M F = f$; in particular, it makes sense for twice continuously differentiable functions $F \in C^2(U_\varepsilon(M))$. In that context, we can also consider just the corresponding tangent directional expressions $B_T^0, B_T^1, B_T^2, A_T^\Xi, \Lambda_T$ and obtain a functional

$$\mathbb{C}_T(F) = B_T^0(F) + B_T^1(F) + B_T^2(F) + A_T^\Xi(F) + \Lambda_T(F).$$

The question is now what we actually loose if we take \mathbb{C}_T of an arbitrary C^2 -function F with $\mathbb{T}_M F = f$ on the ambient space instead of the normal extension $E_N f$. As stated before, the answer to this question can be deduced from Theorem 4.7, and we will discuss this in full detail soon, as we are going to rely heavily on this when it comes to approximation errors later.

But before we come to that, we formalise our previous observations in a couple of definitions to determine the E_N -extrinsic (energy) functionals we will actually consider later: Namely, we want to give a more general description of an E_N -extrinsic functional of the form $\mathbb{C}_M(f) = B_M(f) + \Lambda_M(f) + A_M(f)$. Therein, B_M is roughly speaking the main portion of the functional, so that portion of the functional that is determined by integrals over all of M , while A_M is an auxiliary portion, like the sum over squared function values we have encountered before — but one could also think of some trace on the boundary or on a submanifold of the ESM.

To achieve this more general description, we first define a set $\mathcal{H}_+^\infty(M)$ of suitable weight functions as

$$\mathcal{H}_+^\infty(M) := \bigcup_{n \in \mathbb{N}} \{f \in C^\infty(M, [0, n])\},$$

so the set of all nonnegative bounded functions, and the set of all smooth bounded functions

$$\mathcal{H}^\infty(M) := \bigcup_{n \in \mathbb{N}} \{f \in C^\infty(M, [-n, n])\}.$$

4.57 Definition We call a bilinear functional B_M on $H^2(M)$ an E_N -*extrinsic total functional* if $B_M(f, g) = B_T(E_N f, E_N g)$ and B_T is a bilinear functional for any $F, G \in C^2(U(M))$ or $F = E_N f, G = E_N g$ with $f, g \in H^2(M)$ that has the following form: There is some finite index set I_B such that

$$B_T(F, G) = \sum_{i \in I_B} \int_M \beta_i(F) \beta_i(G).$$

Each $\beta_i(F)$ therein is of the form

$$\beta_i(F) = \beta_i^2(F) + \beta_i^1(F) + \beta_i^0(F),$$

where for a locally smooth and C-bounded tangent frame $T = (\tau^1, \dots, \tau^k)$ as required in the definition of an inverse atlas in $\mathbb{I}(\mathbb{M})$ it holds for each $i \in I_B$ that

1. $\beta_i^0(F) = \eta_i \cdot F$ with $\eta_i \in \mathcal{H}^\infty(\mathbb{M})$,
2. $\beta_i^1(F) = \sum_{j=1}^k \eta_{i,j}^1 \langle \tau^j, \nabla F \rangle$ with $\eta_{i,j}^1 \in \mathcal{H}^\infty(\mathbb{M})$ for each $j = 1, \dots, k$,
3. $\beta_i^2(F) = (\Lambda_i^2(T, H_F))$, where $\Lambda_i^2(T, \cdot)$ maps $M \in \mathbb{R}^{d \times d}$ in the form

$$\Lambda_i^2(T, M) = \sum_{1 \leq j_1, j_2 \leq k} \eta_{j_1, j_2}^{2,i} \cdot ((\tau^{j_1})^t M (\tau^{j_2})),$$

with $\eta_{j_1, j_2}^{2,i} \in \mathcal{H}^\infty(\mathbb{M})$ for any $j_1, j_2 \in \{1, \dots, k\}$.

Directly after the following remark, we will see what the specific choices of those β_i look like in the specific energy functionals we have introduced so far.

4.58 Remark: (1) By conception, any functional of this form is in particular symmetric and positive semidefinite, and also continuous in $H^2(\mathbb{M})$.

(2) Note that the above definition depends on the locally smooth frame T . This means that in general either the transition between such frames needs to be managed or the ESM has to have a globally smooth T . However, for all the specific functionals we have encountered it holds everywhere on \mathbb{M} that the term

$$\sum_{i \in I_B} (\beta_i(F))^2$$

is invariant under rotation of the frame, as it was based on the Euclidean norm of the gradient, the Frobenius norm of the Hessian or on the Laplacian, all of which are invariant under rotations. So in all those cases, we do not have to care about that issue.

4.59 Example:

1. In case of $\mathcal{E}_{\mathbb{H}}^\Xi$, we have that B_T is made up of a sum of k^2 purely second order functionals: For $\ell = i + (j - 1) \cdot k$ and $i, j = 1, \dots, k$ each β_ℓ is of the form

$$\beta_\ell^2(F) = H_F(\tau^i, \tau^j).$$

2. In case of $\mathcal{E}_{\mathbb{H}}^\Xi$, we have that B_T coincides with a η -multiple of that for $\mathcal{E}_{\mathbb{H}}^\Xi$: For $\ell = i + (j - 1) \cdot k$ and $i, j = 1, \dots, k$ each β_ℓ is of the form

$$\beta_\ell^2(F) = \eta H_F(\tau^i, \tau^j).$$

3. In case of \mathcal{E}_{Δ}^Ξ , we have that B_T is only made up of a single second order functional, so the only β_0^2 takes the form

$$\beta_0^2(F) = \sum_{\ell=1}^k H_F(\tau^\ell, \tau^\ell).$$

4. In case of $\mathcal{C}_\Delta^\lambda$ on $M \in \mathbb{M}_{\text{cp}}^k(\mathbb{R}^d)$, there are two equivalent expressions: One is to have for the only $\beta_0(F) = \beta_0^2(F) + \beta_0^1(F) + \beta_0^0(F)$ the choices

$$\beta_0^2(F) = \sum_{\ell=1}^k H_F(\tau^\ell, \tau^\ell) \quad \beta_0^1(F) = 0 \quad \beta_0^0(F) = -\lambda \cdot F$$

while the other is to have $\beta_0 = \beta_0^0$, $\beta_{k+1} = \beta_{k+1}^2$ and for $\ell = 1, \dots, k$ further $\beta_\ell = \beta_\ell^1$ with the choices

$$\beta_0^0(F) = \lambda \cdot F \quad \beta_\ell^1(F) = \sqrt{\lambda} \cdot \langle \tau^\ell, \nabla F \rangle \quad \beta_{k+1}^2(F) = \sum_{\ell=1}^k H_F(\tau^\ell, \tau^\ell).$$

Now that we have formalised the main portion of the functionals we consider, we can turn to the auxilliary portion that augments the main portion.

4.60 Definition Let Ξ be a (possibly empty) finite set of points from $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ and let $k < 4$ in case $\Xi \neq \emptyset$ to ensure continuity of point evaluations. Let $\{\Gamma_i\}_{i \in I_A}$ be a finite (possibly empty) collection of mutually disjoint $\Gamma_i \in \mathbb{M}_{\text{cp}}^{k-1}(\text{clos}(M))$. For weight functions $\eta_i \in \mathcal{H}_+^\infty(\Gamma_i)$, $i \in I_A$, and pointwise weights $\eta_\xi \in \mathcal{H}_\Xi \subseteq]0, \infty[$ we define an *equivalently E_N -extrinsic augmentary functional* by

$$A_M(f, g) = \sum_{\xi \in \Xi} \eta_\xi f(\xi) g(\xi) + \sum_{i \in I_A} \int_{\Gamma_i} \eta_i(f g),$$

for any $f, g \in H^2(M)$. We define correspondingly $A_T(F, G)$ for $F, G \in C^2(U(M))$ or $F = \vec{F} = E_N f$, $G = \vec{G} = E_N g$ by $A_T(F, G) = A_M(T_M F, T_M G)$.

4.61 Remark: (1) These functionals are called "augmentary" because they augment, so they extend, the total functionals in a certain way. Just like the latter, they are symmetric and positive semidefinite by definition. Furthermore, the trace theorem on ESMs and the definition imply that any such augmentary functional $A_M(f, g)$ is continuous on $H^2(M)$.

(2) In case that M has a nonempty boundary and $\Gamma_\ell \cap \partial M \neq \emptyset$ for some ℓ , we actually have to define with $\widehat{M} \in \mathbb{M}_{\text{cp}}^k(\mathbb{R}^d)$ such that $M \Subset \widehat{M}$ and the continuous extension operator $E_M^{\widehat{M}} : H^2(M) \rightarrow H^2(\widehat{M})$ in the general case

$$\int_{\Gamma_\ell} \eta_\ell(f g) := \int_{\Gamma_\ell} \eta_\ell(T_{\Gamma_\ell} E_M^{\widehat{M}} f)(T_{\Gamma_\ell} E_M^{\widehat{M}} g),$$

while for $f, g \in C(\text{clos}(M)) \cap H^2(M)$ we can simply presume the trace to be taken pointwise. That these different approaches yield a well-defined overall definition

can be deduced from the fact that if f_1, f_2 coincide in $H^2(M)$ and $f_1 \in C(\text{clos}(M))$, then $E_M^M f_1 = E_M^M f_2$ and by the trace theorem $T_{\Gamma_\ell} E_M^M f_1 = T_{\Gamma_\ell} E_M^M f_2$, while on the other hand $T_{\Gamma_\ell} f_1$ is continuous.

(3) Of course, we could also include first order directional derivatives of functions on some Γ_ℓ in a similar way for both tangent and M -relative (outer or inner) normal directions, but we omit these for the sake of simplicity — the necessary constructions are obvious. And one could also include other submanifolds of M of presumably higher codimension in a similar way, or relatively compact subdomains of M that are ESMs in their own right.

(4) By construction, it holds for any $F, G \in C^2(U(M))$, $f = T_M F$, $g = T_M G$ and $F = \vec{F} = E_N f$, $G = \vec{G} = E_N g$ that $A_T(F, G) = A_M(f, g) = A_T(\vec{F}, \vec{G})$. And this relation will still hold if one of the enhancements of (3) is performed.

4.62 Example:

1. In case of E_H^Ξ , we have $A_M(f, g) = \sum_{\xi \in \Xi} f(\xi) g(\xi)$.
2. In case of E_η^Ξ , we have that $A_M(f, g) = (1 - \eta) \sum_{\xi \in \Xi} f(\xi) g(\xi)$.
3. In case of E_Δ^Ξ on a compact M , we have again $A_M(f, g) = \sum_{\xi \in \Xi} f(\xi) g(\xi)$.
4. In case of E_Δ^λ , no A_M is present or required. But if we would have e.g. homogeneous Dirichlet boundary conditions for a nonempty smooth boundary Γ of $M \in \mathbb{M}_{\text{sd}}^k(\mathbb{R}^d)$, then these can lead to the form

$$A_M(f, g) = \int_{\Gamma} f g.$$

Finally, we will formalise the linear portion of the functionals. In that, we will restrict ourselves to linear functionals that appear as the linear portions of quadratic functionals B_M^ℓ and / or A_M^ℓ when applied to $f - g_\ell$ for suitable fixed g_ℓ , and speak of linear functionals *subordinate to* B_M^ℓ and A_M^ℓ .

4.63 Definition 1. Let A_M be an augmentary E_N -extrinsic functional on $H^2(M)$, based on Ξ and $\{\Gamma_i\}_{i \in I_A}$, weights $\{\eta_\xi\}_{\xi \in \Xi}$ and weight functions $\{\eta_i\}_{i \in I_A}$. A linear functional Λ_A on $H^2(M)$ is called E_N -extrinsic subordinate to A_M if there are $\Xi_A \subseteq \Xi$ and $J_A \subseteq I_A$ such that for suitable choices of function values $\gamma_\xi \in \mathbb{R}$ and functions $g_j \in H^{\frac{3}{2}}(\Gamma_j)$ the functional Λ_A is the linear part of

$$\sum_{\xi \in \Xi_A} \eta_\xi (f(\xi) - \gamma_\xi)^2 + \sum_{j \in J_A} \int_{\Gamma_j} \eta_j (f - g_j)^2.$$

2. Let B_M be an E_N -extrinsic quadratic total functional on $H^2(M)$ with associated index set I_B . A linear functional Λ_B on $H^2(M)$ is called E_N -extrinsic subordinate to

B_M if there is an index set $J_B \subseteq I_B$ such that for suitable functions $\vec{G}_j = E_N g_j$ with $g_j \in H^2(M)$, $j \in J_B$, its tangent directional version $\Lambda_{B,T}$ is the linear part of

$$\sum_{j \in J_B} \int \beta_j(F - \vec{G}_j) \beta_j(F - \vec{G}_i).$$

3. Finally, we say that a linear functional Λ_M on $H^2(M)$ with corresponding tangent directional Λ_T is E_N -extrinsic subordinate to $A_M + B_M$ if it is the sum of two linear functionals Λ_A and Λ_B that are either the zero functional or E_N -extrinsic subordinate to A_M and B_M , respectively. This is denoted in future by $\Lambda_M \in \mathbb{L}_M(A_M, B_M)$.

4.64 Remark: (1) Such functional is continuous on the space $H^2(M)$ by definition. (2) In particular, it is clear by this definition that there is a fixed value $\varepsilon_\Lambda \geq 0$ such that for any $f \in H^2(M)$ with $\vec{F} = E_N f$ or $f = T_M F$, $F \in C^2(U(M))$ it holds *simultaneously* that both

$$\mathcal{E}_T(\vec{F}) = B_T(\vec{F}) + \Lambda_T(\vec{F}) + A_T(\vec{F}) + \varepsilon_\Lambda \geq 0, \quad \mathcal{E}_T(F) = B_T(F) + \Lambda_M(F) + A_M(F) + \varepsilon_\Lambda \geq 0.$$

This property is retained for any larger choice of ε_Λ .

4.65 Example:

1. In case of \mathcal{E}_H^Ξ , we have $\Lambda_T = 0$ and therefore any $\varepsilon_\Lambda \geq 0$ is valid.
2. In case of \mathcal{E}_η^Ξ , we have that

$$\Lambda_T(F) = -2(1 - \eta) \sum_{\xi \in \Xi} F(\xi) \gamma_\xi,$$

and thus we have to require

$$\varepsilon_\Lambda \geq (1 - \eta) \sum_{\xi \in \Xi} (\gamma_\xi)^2.$$

3. In case of $\mathcal{E}_\Delta^\lambda$ on a compact M , we have again $\Lambda_T = 0$ and so any $\varepsilon_\Lambda \geq 0$ is valid.

4.66 Definition An equivalently E_N -extrinsic $\mathcal{E}_M = B_M + \Lambda_M + A_M$ with total B_M , augmentary A_M and linear $\Lambda_M \in \mathbb{L}_M(A_M, B_M)$ is called an *augmented E_N -extrinsic functional* and denoted by $\mathcal{E}_M \in \mathbb{E}_N(M)$.

If $\Lambda_M = 0$, then $\mathcal{E}_M(f)$, $\mathcal{E}_T(f)$ are derived from a bilinear functional $\mathcal{E}_M(f, g)$, $\mathcal{E}_T(f, g)$ that is consequently called an *augmented bilinear E_N -extrinsic functional*. In that case, we denote this fact by $\mathcal{E}_M \in \mathbb{E}_N^B(M)$.

As stated before, the tangent directional version \mathcal{E}_T of an augmented E_N -extrinsic functional $\mathcal{E}_M = B_M + \Lambda_M + A_M \in \mathbb{E}_N(M)$ has a more general meaning for functions in $C^2(U(M))$ even if they are not normal extensions. Consequently, it is interesting

to investigate the deviation $\mathcal{E}_T(F - \vec{F})$ for $\vec{F} = E_N(\mathbb{T}_M F)$ and $F \in C^2(U(M))$, as this gives us insight into the deviation from the intrinsic functional value and will be very useful in proving upcoming results.

In doing that, we restrict ourselves first to the case $\Lambda_M = 0$ and ignore also anything in \mathcal{E}_T except for the squared purely second order terms, so the part

$$B_T^2(F) = \int_M \sum_{i \in I_B} (\beta_i^2(F))^2.$$

This is possible because by construction for any F it holds $\beta_i^j(F - \vec{F}) = 0$ for any $i \in I_B$ and $j = 0, 1$, and by construction $A_T(F - \vec{F}) = 0$. In order to simplify the notation and arguments, we suppose in the following discussion that $|I_B| = 1$. We will see afterwards that finite summation has no relevant effect, and this restriction allows us to omit a couple of indices. So we reduce the discussion to

$$\beta^2(F) = \sum_{1 \leq i, j \leq k} \eta_{ij} H_F(\tau^i, \tau^j).$$

Recalling the results of Theorem 4.7 and its proof, we can directly deduce that it holds pointwise for any $x \in M$

$$\left| \sum_{ij} \eta_{ij} (H_F(x)(\tau^i, \tau^j) - H_{\vec{F}}(x)(\tau^i, \tau^j)) \right| \leq c \|\nabla_N F(x)\|_2.$$

We can thus also conclude that

$$\left| \sum_{ij} \eta_{ij} (H_F(x)(\tau^i, \tau^j) - H_{\vec{F}}(x)(\tau^i, \tau^j)) \right|^2 \leq c \|\nabla_N F(x)\|_2^2.$$

Taking integrals gives us

$$B_T^2(F - \vec{F}) \leq c \int_M \|\nabla_N F\|_2^2.$$

As this works out for all summands in case $|I_B| > 1$, we can instantly draw the following conclusion:

4.67 Conclusion For an ESM $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ and an augmented E_N -extrinsic functional $\mathcal{E}_M = B_M + A_M \in \mathbb{E}_N^g(M)$ on $H^2(M)$ with corresponding tangent Euclidean expression \mathcal{E}_T it holds for any $f \in C^2(M)$, $F \in C^2(U(M))$ with $f = \mathbb{T}_M F$ and $\vec{F} = E_N f$ that

$$\mathcal{E}_T(F - \vec{F}) \leq c \|\nabla_N F\|_{L_2(M)}^2.$$

Actually, we can even bound $B_T(F, G)$ and $A_T(F, G)$ for two functions F, G such that

both $B_T(F), B_T(G)$ and $A_T(F), A_T(G)$ are with well-defined and finite: We can apply the usual Cauchy-Schwarz inequalities for $L_2(\mathcal{M})$, for $L_2(\Gamma_\ell)$ for arbitrary ℓ or for Euclidean space (in case of $\Xi \neq \emptyset$) to deduce

$$B_T(F, G) \leq c \sqrt{B_T(F)} \cdot \sqrt{B_T(G)}, \quad A_T(F, G) \leq \sqrt{A_T(F)} \cdot \sqrt{A_T(G)}.$$

In particular, this allows us to deduce in the light of the previous conclusion that for any admissible choice of G it holds

$$B_T(F - \vec{F}, G) \leq c \|\nabla_N F\|_2 \sqrt{B_T(G)}, \quad A_T(F - \vec{F}, G) = 0.$$

Again, we sum this up in a conclusion for future referencing:

4.68 Conclusion Let $\mathcal{M} \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ and let $f \in C^2(\mathcal{M})$. Let $F \in C^2(U(\mathcal{M}))$ with $f = T_{\mathcal{M}}F$ and let $\vec{F} = E_N f$. Let G_1, G_2 be either in $C^2(U(\mathcal{M}))$ or normal extensions of functions in $H^2(\mathcal{M})$ for $i = 1, 2$. Then it holds for any augmented E_N -extrinsic functional $\mathcal{E}_{\mathcal{M}} \in \mathbb{E}_N^{\mathfrak{a}}$ with $\mathcal{E}_T = B_T + A_T$ that

$$\mathcal{E}_T(F - \vec{F}, G_1) \leq c \|\nabla_N F\|_2 \sqrt{B_T(G_1)}.$$

Finally, the same arguments as applied before give us that for a linear functional Λ_B subordinate to some $B_{\mathcal{M}}$ and corresponding tangent Euclidean $\Lambda_{B,T}$ it holds by Cauchy-Schwarz

$$|\Lambda_{B,T}(F - \vec{F})| \leq c \|\nabla_N F\|_2,$$

while for Λ_A this difference functional is directly clear to vanish. Thus we obtain:

4.69 Conclusion Let $\mathcal{M} \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ and let $B_{\mathcal{M}} + A_{\mathcal{M}} \in \mathbb{E}_N^{\mathfrak{a}}(\mathcal{M})$ with corresponding tangent Euclidean expressions B_T, A_T . Let $f \in C^2(\mathcal{M})$, $F \in C^2(U(\mathcal{M}))$ with $f = T_{\mathcal{M}}F$ and $\vec{F} = E_N f$. Let $\Lambda_{\mathcal{M}} \in \mathbb{L}_{\mathcal{M}}(A_{\mathcal{M}}, B_{\mathcal{M}})$ be subordinate to $B_{\mathcal{M}} + A_{\mathcal{M}}$. Then it holds

$$|\Lambda_T(F - \vec{F})| \leq c \|\nabla_N F\|_2.$$

Chapter 5

Ambient Functional Approximation Methods

In this chapter we are going to revise the tangential energy functionals from an approximation theoretic point of view: Directly accessing the tangential form of intrinsic functionals with normal extensions is almost hopeless when all you have is some finite dimensional space of functions like TP-splines. Consequently, we will have to consider approximations to these functionals, best accompanied by some error analysis and convergence results, both of which will be provided in this chapter. In the course of this, we will rely on *augmented E_N -extrinsic (energy) functionals* and state most results for these to obtain some generality. The specific treatment of our concrete examples of energy functionals is left for later chapters.

To be more precise, we will introduce a general, penalty-based approximation method for various situations, all of which can be exemplified by some of our particular energy functionals: First, we will have a look at energy minimisation in convex sets with the obvious example of C_H^Ξ . Then we will turn to situations where the functional is already applied to a residual, so $C(f - f_0)$, motivated by the solution of an elliptic PDE with $C_\Delta^\lambda(f - f^*)$. Only after we have exemplified the basic structure of the necessary argumentation in these important examples, we will turn to the most general situation where $\Lambda_M \neq 0$, as exemplified by C_η^Ξ in particular.

In the course of this, we will demand that M is equipped with the normal foliation and thus gives rise to the normal extension, with a suitable $U(M)$ as its result. We also demand that we can extend (normal) frames on M into this neighbourhood along the normals by taking the frame in the closest point. Both demands mean actually no restriction, as we had seen in the second chapter.

The reader can further bear in mind that one could replace this normal extension by any other orthogonal extension, provided we can also access the respective frames implied by the trajectories of this other extension in the ambient space.

But for the sake of simplicity, we restrict ourselves here to the particular case of normal extensions, foliations and frames.

When it comes to the practical requirements we demand from the representation of the ESM, then it turns out that these have quite a broad scope: We need only a representation of M that allows some kind of numerical integration and provides approximate normals as well — where of course the density and quality of the approximations of both M and its normals have a direct impact on the quality of the result. So essentially, even a dense point cloud with corresponding normals, and integration performed by simple Riemannian sums, would suffice.

5.1 Penalty Approximation in Functional Optimisation

We are now going to approach the problem of intrinsic functional minimisation by penalty approximation. The objective of the penalty is fairly obvious by the last section of the previous chapter: We have to force the normal derivatives to approach zero. So for $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ we turn now to an arbitrary augmented E_N -extrinsic energy functional $\mathcal{E}_M : H^2(M_0) \rightarrow \mathbb{R}$ with $\mathcal{E}_M(f) = B_M(f) + \Lambda_M(F) + A_M(f)$ on some $M_0 \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ with $M_0 \Subset M$ and (possibly empty) boundary Γ_0 such that \mathcal{E}_M has corresponding tangent directional expression \mathcal{E}_T of the form

$$\mathcal{E}_T(F) = B_T(F) + \Lambda_T(F) + A_T(F).$$

Then we define the *Ambient Penalty Approximation* (APA) functional with penalty exponents $\sigma_M, \sigma_C \geq 0$ on M_0 for S from the spline space $S_h^m(C_h(M_0))$ as

$$P(S, \sigma_M, \sigma_C) := \mathcal{E}_T(S) + \Lambda_T(S) + h^{-\sigma_M} N_M^\nabla(S, M_0) + h^{-\sigma_C} N_C^\nabla(S, M_0) \rightarrow \min!$$

where we set

$$N_M^\nabla(S, M_0) := \int_{M_0} \|\nabla_N S\|_2^2 \quad \text{and} \quad N_C^\nabla(S, M_0) := \int_{C_h(M_0)} \|\nabla_N S\|_2^2.$$

Therein, we understand again $\nabla_N S(x)$ for $x \notin M$ as the projection of the gradient to the normal space of the closest point of x on M , so $N = N(\Pi_M(x))$. This is also the reason why we have to demand $M_0 \Subset M$: We need to have this projection well-defined at least for sufficiently small $h > 0$ on all active cells. Otherwise, we might have cells where this projection is not well-defined even for $h \rightarrow 0$, and we wish to avoid this problem for its technical complexity. Of course, if M_0 itself has no boundary, then clearly we have $M_0 = M$. Otherwise, we have for such

$\mathbf{M}_0 \in \mathbb{M}_{\text{sd}}^k(\mathbb{R}^d)$ a boundary that is made up of finitely many $(k - 1)$ -dimensional compact ESMs.

5.1 Remark: We will state all our results for TP-splines as the approximation space that is applied. However, the use of TP-splines is actually just exemplary; we simply felt that a general formulation would have introduced further difficulties in some of the statements. In particular, the "space penalty"

$$h^{-\sigma_C} N_C^\nabla(S, \mathbf{M}_0) = h^{-\sigma_C} \int_{C_h(\mathbf{M}_0)} \|\nabla_N S\|_2^2$$

is something that was tailored for splines to avoid certain problems with the stability of some large linear system that appears in practical implementations. Some other approximation methods might make use of it as well, while others will presumably not do so. But we carry this along in the present chapter because we want to emphasise that it has no negative impact on the approximation results for suitable penalty exponents. In particular a valid choice will always be $\sigma_C = \sigma_M$, as we have seen when we discussed splines: We found in Remark 3.41 that we can expect the convergence rate of the normal derivative on $C_h(\mathbf{M}_0)$ to be at least the convergence rate of the normal derivative on \mathbf{M} itself.

5.2 Important: In the following arguments, we will omit the distinction between \mathbf{M} and \mathbf{M}_0 for the sake of simplicity, as it plays no crucial role in the argumentation. In particular, we will therefore omit the integration domain in $N_M^\nabla(S, \mathbf{M}_0)$ and $N_C^\nabla(S, \mathbf{M}_0)$, and just write

$$N_M^\nabla(S) := \int_{\mathbf{M}} \|\nabla_N S\|_2^2 \quad \text{and} \quad N_C^\nabla(S) := \int_{C_h(\mathbf{M})} \|\nabla_N S\|_2^2.$$

However, the reader should bear in mind that in practice, this distinction is absolutely crucial if \mathbf{M}_0 has nonempty boundary. We further omit the distinction between σ_C and σ_M , as $\sigma_C = \sigma_M$ will always be valid, and postpone the discussion of specific choices to the practical examples presented later.

Regarding the unique solvability of the APA minimisation problem, we will now restrict ourselves to the case of a strictly convex and coercive augmented E_N -extrinsic functional, as mere augmented E_N -extrinsic functionals do not necessarily have unique minimisers on convex subsets of H^2 . In some explicitly stated situations we will however draw conclusions also for some more general situations. Now, we first consider the case $\Lambda_M = 0$ and have

$$P(S, \sigma) := E_T(S) + h^{-\sigma} N_M^\nabla(S) + h^{-\sigma} N_C^\nabla(S).$$

Then we can directly see that this is a quadratic functional on the finite dimen-

sional spline space, implied by a suitable inner product; bilinearity and symmetry of the corresponding bilinear formulation are obvious, and the positive definiteness can be seen as follows: If the functional vanishes, both penalty terms vanish in particular. And for all functions where this holds, the component $\mathcal{E}_T(S_h)$ vanishes precisely if the argument is zero. Consequently, we have a positive definite quadratic functional on a finite dimensional space, the spline space. The addition of an additional continuous linear functional Λ_M does no harm to the existence of a minimum there, and so the existence of a unique minimiser is clear also in the general case with nonvanishing linear Λ_M . Summing these arguments up, we obtain the following theorem:

5.3 Theorem *Any APA functional based on a continuous, elliptic bilinear functional $B_M + A_M \in \mathbb{E}_N^{\mathbf{r}}(M)$ and linear $\Lambda_M \in \mathbb{L}_M(A_M, B_M)$ has a unique minimiser in the space $S_h^m(C_h(M))$.*

We are now going to present a sequence of theorems dealing with different situations of (augmented) equivalently E_N -extrinsic (energy) functionals. In the first results, making up the first two subsections to follow, we will demand that the linear part of the functional is zero. This reduces the complexity in the respective proofs substantially, and we shall only drop this restriction in the very end, when we have clarified the structure of argumentation in the other cases.

In all situations, we will demand the splines to be at least of order four, so in particular to be twice continuously differentiable. We further demand that there is a family $(s_h^*)_{h < h_0}$ of restrictions of functions $(S_h^*)_{h < h_0}$ from $S_h^m(C_h(M))$ such that for the functional optimum $f^* \in H^{\varrho}(M)$ with $\varrho \geq 2$ and some $\beta_0, \beta_1, \beta_2 > 0$ it holds

$$\begin{aligned} \|\nabla_N S_h^*\|_2^2_{L_2(C_h(M))} &\leq c h^{\beta_0} \|f^*\|_{H^{\varrho}(M)}^2, \\ \|\nabla_N S_h^*\|_2^2_{L_2(M)} &\leq c h^{\beta_1} \|f^*\|_{H^{\varrho}(M)}^2, \\ \|s_h^* - f^*\|_{H^2(M)}^2 &\leq c h^{\beta_2} \|f^*\|_{H^{\varrho}(M)}^2. \end{aligned}$$

This will be abbreviated as $(S_h^*)_{h < h_0} \in \text{App}(f^*, \varrho, \beta_0, \beta_1, \beta_2)$.

5.4 Remark: (1) Recalling Sections 3.3.4 and 3.3.5, we can give explicit values for the approximation orders $\beta_0, \beta_1, \beta_2$. As these depend on the actual regularity of the optimum f^* , we chose the general formulation by $\text{App}(f^*, \varrho, \beta_0, \beta_1, \beta_2)$ to deal with various cases, subcases and so on. The reader can, however, bear in mind that with sufficient regularity of the solution, i.e. $f^* \in H^m(M)$, the respective values are simply $\beta_0 \geq m - 1$, $\beta_1 = m - 1$, $\beta_2 = m - 2$.

(2) As we have stated in Remark 3.41, any β_1 is in particular a valid choice for β_0 , so we omit the latter in our theoretical arguments: We can simply suppose $\beta_0 = \beta_1$, deal with any other $\beta_0 < \beta_1$ right in the same way and leave the exact investigation

of the impact of β_0 on the stability for later research. This situation shall then be abbreviated by $(S_h^*)_{h < h_0} \in \text{App}(f^*, \varrho, \beta_1, \beta_2)$.

(3) In practice, it might be hard to determine the set $C_h(\mathbb{M})$ of cells active on \mathbb{M} without risking to “miss” a relevant cell. So it may also be appropriate to use $C_h(U_h(\mathbb{M}))$ or another more convenient superset $\widehat{C}_h(\mathbb{M})$ of $C_h(\mathbb{M})$ for the “space penalty”. This bears less danger of missing a relevant cell that is active on \mathbb{M} and it does no harm to the approximation power, if the relation

$$\|\nabla_N S_h^*\|_{L_2(C_h(\mathbb{M}))}^2 \leq c h^{\beta_0} \|f^*\|_{H^\varrho(\mathbb{M})}^2$$

is replaced by corresponding

$$\|\nabla_N S_h^*\|_{L_2(\widehat{C}_h(\mathbb{M}))}^2 \leq c h^{\beta_0} \|f^*\|_{H^\varrho(\mathbb{M})}^2.$$

(4) In any of the upcoming convergence results, arguments will remain valid with only small changes for other approximating families $(F_h^*)_{0 < h < h_0}$ of C^2 -functions with traces $(f_h^*)_{0 < h < h_0}$ as long as the penalty functional is stable and it holds

$$\|\nabla_N F_h^*\|_{L_1(\mathbb{M})}^2 \leq c h^{\beta_1} \|f^*\|_{H^\varrho(\mathbb{M})}^2, \quad \|f_h^* - f^*\|_{H^2(\mathbb{M})}^2 \leq c h^{\beta_2} \|f^*\|_{H^\varrho(\mathbb{M})}^2.$$

These can, as in our exemplary spline case, be extended by additional demands that stabilise the process — as long as those do no harm to the approximation orders required above.

5.2 Penalty Approximation for Energies in Convex Sets

In the following theorem we are now going to present a first convergence result, deducing a convergence order for APA minimisation from the best possible order of approximation; it aims at the specific functionals $\mathcal{E}_H^\Xi(\cdot)$ and $\mathcal{E}_\Delta^\Xi(\cdot)$ in particular. Here and in the following, we will always understand $\mathcal{E}_\mathbb{M}(F)$ as $\mathcal{E}_\mathbb{M}(\mathbb{T}_\mathbb{M}F)$ when F is a function defined on the ambient space. This is valid at least for functions of the form $E_N f$ for $f \in H^2(\mathbb{M})$ or functions $F \in C^2(U(\mathbb{M}))$, and these are the only situations we will encounter.

5.5 Theorem *Let $\mathbb{M} \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ and let $\mathcal{E}_\mathbb{M} = B_\mathbb{M} + A_\mathbb{M} \in \mathbb{E}_N^\mathfrak{a}(\mathbb{M})$ be an augmented elliptic functional on $H^2(\mathbb{M})$. Let $f^* \in H^\varrho(\mathbb{M})$ be the minimiser of $\mathcal{E}_\mathbb{M}$ in the convex set $D_{\text{co}} \subseteq H^2(\mathbb{M})$. Let $(s_h^*)_{h < h_0}$ be a family of restrictions of approximations $(S_h^*)_{h < h_0} \in \text{App}(f^*, \varrho, \beta_1, \beta_2)$ such that $s_h^* \in D_{\text{co}}$ for any $0 < h < h_0$. Then $P(\cdot, \sigma)$ has a unique minimiser S_h in D_{co} for any $0 < h < h_0$ and arbitrary $0 < \sigma < \beta_1$. The trace $s_h = \mathbb{T}_\mathbb{M} S_h$ of this minimiser satisfies the relation*

$$\|s_h - f^*\|_{H^2(\mathcal{M})} \leq c h^\alpha \|f^*\|_{H^e(\mathcal{M})}^2$$

for $\alpha = \min\{\sigma/2, \beta_2/2, \beta_1 - \sigma\}$ and a constant c independent of f^* .

Proof: We write as usual \mathcal{E}_T for the formulation of \mathcal{E}_M in terms of derivatives in tangent directions. By the optimality of S_h we obtain

$$\mathcal{E}_T(S_h) + h^\sigma N_M^\nabla(S_h) + h^\sigma N_C^\nabla(S_h) \leq \mathcal{E}_T(S_h^*) + h^\sigma N_M^\nabla(S_h^*) + h^\sigma N_C^\nabla(S_h^*). \quad (5.5.1)$$

Furthermore, we can conclude by symmetry and bilinearity that for $\vec{S}_h^* = E_N s_h^*$ due to Cauchy-Schwarz inequality and Conclusion 4.67

$$\begin{aligned} \mathcal{E}_T(S_h^*) &= \mathcal{E}_T(S_h^* - \vec{S}_h^* + \vec{S}_h^*) = \mathcal{E}_T(\vec{S}_h^*) + \mathcal{E}_T(S_h^* - \vec{S}_h^*) + 2\mathcal{E}_T(S_h^* - \vec{S}_h^*, \vec{S}_h^*) \\ &\leq \mathcal{E}_M(\vec{S}_h^*) + 2\sqrt{\mathcal{E}_M(\vec{S}_h^*)}\sqrt{\mathcal{E}_T(S_h^* - \vec{S}_h^*)} + \mathcal{E}_T(S_h^* - \vec{S}_h^*) \\ &\leq \mathcal{E}_M(\vec{S}_h^*) + c\sqrt{\mathcal{E}_M(\vec{S}_h^*)}\sqrt{N_M^\nabla(S_h^*)} + cN_M^\nabla(S_h^*). \end{aligned} \quad (5.5.2)$$

By the conception of S_h^* we know that $N_M^\nabla(S_h^*) \leq c h^{\beta_1} \|f^*\|_{H^e(\mathcal{M})}^2$. Since additionally for $h \rightarrow 0$ it holds $s_h^* \rightarrow f^*$ in $H^2(\mathcal{M})$, and \mathcal{E}_M is continuous in the standard H^2 -norm, we have

$$\mathcal{E}_M(\vec{S}_h^*) \leq c \|s_h^*\|_{H^2(\mathcal{M})}^2 \leq c \|f^*\|_{H^e(\mathcal{M})}^2,$$

because by the triangle inequality

$$\|s_h^*\|_{H^2(\mathcal{M})} \leq c h^{\beta_2} \cdot \|f^*\|_{H^e(\mathcal{M})} + \|f^*\|_{H^2(\mathcal{M})} \leq c \|f^*\|_{H^e(\mathcal{M})}.$$

Consequently, we obtain by insertion into (5.5.1) that

$$\mathcal{E}_T(S_h) + h^\sigma N_M^\nabla(S_h) + h^\sigma N_C^\nabla(S_h) \leq c \|f^*\|_{H^e(\mathcal{M})}^2.$$

So in particular

$$N_M^\nabla(S_h) \leq c h^\sigma \|f^*\|_{H^e(\mathcal{M})}^2 \quad \text{and} \quad \mathcal{E}_T(S_h) \leq c \|f^*\|_{H^e(\mathcal{M})}^2.$$

Now let us investigate $\mathcal{E}_T(S_h)$ further. Once again we see by symmetry, bilinearity, Cauchy-Schwarz and Conclusion 4.67 that

$$\begin{aligned} \mathcal{E}_T(S_h) &= \mathcal{E}_T(S_h - \vec{S}_h + \vec{S}_h) = \mathcal{E}_T(\vec{S}_h) + \mathcal{E}_T(S_h - \vec{S}_h) + 2\mathcal{E}_T(S_h - \vec{S}_h, \vec{S}_h) \\ &= \mathcal{E}_M(S_h) + \mathcal{E}_T(S_h - \vec{S}_h) + 2\mathcal{E}_T(S_h - \vec{S}_h, \vec{S}_h) \\ &\geq \mathcal{E}_M(S_h) + \mathcal{E}_T(S_h - \vec{S}_h) - 2\sqrt{\mathcal{E}_M(\vec{S}_h)}\sqrt{\mathcal{E}_T(S_h - \vec{S}_h)} \\ &\geq \mathcal{E}_M(S_h) - 2\sqrt{\mathcal{E}_M(\vec{S}_h)}\sqrt{\mathcal{E}_T(S_h - \vec{S}_h)} \\ &\geq \mathcal{E}_M(S_h) - c\sqrt{\mathcal{E}_M(S_h)}\sqrt{N_M^\nabla(S_h)}. \end{aligned}$$

So we can deduce that by our assumptions on $N_M^\nabla(S_h)$ it holds

$$\mathcal{E}_T(S_h) \geq \mathcal{E}_M(S_h) - c \sqrt{\mathcal{E}_M(S_h)} \cdot h^{\sigma/2} \|f^*\|_{H^e(M)}. \quad (5.5.3)$$

This gives us by some simple restructurings

$$\begin{aligned} \mathcal{E}_M(S_h) &\leq \mathcal{E}_T(S_h) + c \sqrt{\mathcal{E}_M(S_h)} \cdot h^{\sigma/2} \|f^*\|_{H^e(M)} \\ &\leq c \|f^*\|_{H^e(M)}^2 + c \sqrt{\mathcal{E}_M(S_h)} \cdot h^{\sigma/2} \|f^*\|_{H^e(M)}. \end{aligned}$$

Thereby we must have that $\mathcal{E}_M(S_h) \leq c \|f^*\|_{H^e(M)}^2$. To see this, we apply standard calculus for quadratic equations and conclude that the above inequality implies

$$\sqrt{\mathcal{E}_M(S_h)} \leq c \cdot \left(h^{\sigma/2} \|f^*\|_{H^e(M)} \pm \sqrt{h^\sigma \|f^*\|_{H^e(M)}^2 + 4 \|f^*\|_{H^e(M)}^2} \right) \leq c \|f^*\|_{H^e(M)}. \quad (5.5.4)$$

We conclude thereby and by

$$\begin{aligned} \mathcal{E}_T(S_h) &\leq \mathcal{E}_T(S_h^*) + h^{-\sigma} N_M^\nabla(S_h^*) + h^{-\sigma} N_C^\nabla(S_h^*) \\ &\leq \mathcal{E}_M(S_h^*) + c \sqrt{\mathcal{E}_M(\vec{S}_h^*)} \sqrt{N_M^\nabla(S_h^*)} + c N_M^\nabla(S_h^*) + h^{-\sigma} N_M^\nabla(S_h^*) + h^{-\sigma} N_C^\nabla(S_h^*) \\ &\leq \mathcal{E}_M(S_h^*) + c \|f^*\|_{H^e(M)} \sqrt{N_M^\nabla(S_h^*)} + c N_M^\nabla(S_h^*) + h^{-\sigma} N_M^\nabla(S_h^*) + h^{-\sigma} N_C^\nabla(S_h^*) \\ &\leq \mathcal{E}_M(S_h^*) + c h^{\beta_2/2} \|f^*\|_{H^e(M)}^2 + c h^{\beta_1-\sigma} \|f^*\|_{H^e(M)}^2 + c h^{\beta_1-\sigma} \|f^*\|_{H^e(M)}^2 \end{aligned} \quad (5.5.5)$$

that because $\sigma < \beta_1$ we obtain via insertion of (5.5.5) into (5.5.3)

$$\mathcal{E}_M(S_h) \leq \mathcal{E}_M(S_h^*) + c (h^{\sigma/2} + h^{\beta_1-\sigma}) \|f^*\|_{H^e(M)}^2.$$

We now subtract $\mathcal{E}_M(\vec{F}^*)$ on both sides and obtain

$$0 \leq \mathcal{E}_M(S_h) - \mathcal{E}_M(\vec{F}^*) \leq \mathcal{E}_M(S_h^*) - \mathcal{E}_M(\vec{F}^*) + c (h^{\sigma/2} + h^{\beta_1-\sigma}) \|f^*\|_{H^e(M)}^2.$$

Since $\mathcal{E}_M(\cdot)$ was continuous and elliptic, its square root gives us an equivalent norm on $H^2(M)$, and we can apply the triangle inequality. Consequently by the (inverse) triangle inequality and the minimality of $\mathcal{E}_M(\vec{F}^*)$

$$\sqrt{\mathcal{E}_M(S_h^*)} - \sqrt{\mathcal{E}_M(\vec{F}^*)} \leq c \|s_h^* - f^*\|_{H^2(M)} \leq c h^{\beta_2/2} \|f^*\|_{H^e(M)}.$$

Because we can further directly conclude from the minimality of f^* and the continuity of \mathcal{E}_M that

$$\sqrt{\mathcal{E}_M(S_h^*)} + \sqrt{\mathcal{E}_M(\vec{F}^*)} \leq 2\sqrt{\mathcal{E}_M(S_h^*)} \leq c \|f^*\|_{H^e(M)},$$

we obtain by the third binomial

$$0 \leq \mathcal{E}_M(S_h^*) - \mathcal{E}_M(\vec{F}^*) \leq c h^{\beta_2/2} \|f^*\|_{H^e(M)}^2.$$

Therefore we reach thanks to $\mathcal{E}_M(S_h) \geq \mathcal{E}_M(\vec{F}^*)$ our final goal via

$$|\mathcal{E}_M(S_h) - \mathcal{E}_M(\vec{F}^*)| = \mathcal{E}_M(S_h) - \mathcal{E}_M(\vec{F}^*) \leq c (h^{\beta_2/2} + h^{\sigma/2} + h^{\sigma-\beta_1}) \|f^*\|_{H^e(M)}^2$$

by application of Conclusion 4.56. \square

5.6 Remark: (1) With β_1 and β_2 known explicitly due to the third chapter, one can directly calculate a minimizer for the upper bound on the convergence w.r.t. σ . However, we will later find that in practice there is actually even a better choice. (2) Most importantly, this result applies to $\mathcal{E}_H^\Xi(\cdot)$ of Theorem 4.49 and to $\mathcal{E}_\Delta^\Xi(\cdot)$ of Cor. 4.52. For these, the fixed interpolation constraints for Ξ that define D_{co} imply that the sum of function values that makes up augmentary A_M remains constant. So the functionals reduce to be effectively just $\mathcal{E}_M(\cdot) = \mathcal{E}_H(\cdot)$ and $\mathcal{E}_M(\cdot) = \mathcal{E}_\Delta(\cdot)$, respectively.

The previous result is valid in convex sets D_{co} if we can guarantee that all functions come from that set. Unfortunately, it can be hard to achieve this for finite dimensional spaces like the spline space: If one does not have finite interpolation constraints, but for example a homogeneous Dirichlet condition on some submanifold $\Gamma \in \mathbb{M}_{cp}^{k-1}(M)$ or $\Gamma = \partial M \in \mathbb{M}_{cp}^{k-1}(\mathbb{R}^d)$, then any attempt to satisfy these exactly with TP-splines will usually be in vain. To overcome this, it can be beneficial to include the conditions into the penalty.

To achieve that, we will now suppose that we have an E_N -extrinsic functional $\mathcal{E}_M \in \mathbb{E}_N^\alpha(M)$ with or without augmentary portion, and not necessarily elliptic. And we demand that $D_{co} \subseteq H^2(M)$ is characterised via some suitable augmentary functional

$$A_M^{co}(f, g) = \sum_{\xi \in \Xi} \eta_\xi f(\xi) g(\xi) + \sum_{\ell \in I_A} \int_{\Gamma_\ell} \eta_\ell f g$$

for a suitable choice of a function $g_{co} \in H^2(M)$ with $g_{co} \in C(M)$ if $\Xi \neq \emptyset$ in the form

$$D_{co} := \left\{ f \in H^2(M) : A_M(f - g_{co}) = \sum_{\xi \in \Xi} \eta_\xi (f(\xi) - g_{co}(\xi))^2 + \sum_{\ell \in I_A} \int_{\Gamma_\ell} \eta_\ell (f - g_{co})^2 = 0 \right\}.$$

Thereby we introduce the modified penalty functional $P_{co}(S_h, \sigma, \sigma_{co})$ as

$$P_{co}(S, \sigma, \sigma_{co}) = \mathcal{E}_T(S) + h^{-\sigma_{co}} A_M(S - E_N g_{co}) + h^{-\sigma} N_M^\nabla(S) + h^{-\sigma} N_C^\nabla(S).$$

We can then consider $\mathcal{E}_M + A_M^{co}$ again as an (energy) functional, and as long as $\mathcal{E}_M + A_M^{co}$ is elliptic, the unique solvability of the penalty minimisation problem and the existence of a minimiser remain unaffected.

As usual, the actual choice of penalty exponent σ_{co} is delicate therein. And while we cannot apply our previous arguments on convergence, because we have to include the additional penalty into our considerations, we still have something more or less satisfactory, though of course weaker:

5.7 Theorem *Let $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ and let $D_{\text{co}} \subseteq H^2(M)$ be a closed, convex set, characterised by $A_M^{\text{co}}(f - g_{\text{co}}) = 0$ as introduced above. Let \mathcal{E}_M be a bilinear E_N -extrinsic functional on $H^2(M)$ such that $\mathcal{E}_M^{\text{co}} = \mathcal{E}_M + A_M^{\text{co}} \in \mathbb{E}_N^{\text{r}}(M)$ is elliptic. Let $f^* \in H^2(M)$ be the minimiser of \mathcal{E}_M in D_{co} . Let $(s_h^*)_{h < h_0}$ be a family of restrictions of approximations $(S_h^*)_{h < h_0} \in \text{App}(f^*, \varrho, \beta_1, \beta_2)$ such that for some suitable $\beta_{\text{co}} \geq \beta_2$ and any $0 < h < h_0$ additionally*

$$A_M^{\text{co}}(s_h^* - g_{\text{co}}) \leq c h^{\beta_{\text{co}}} \|f^*\|_{H^2(M)}^2.$$

Then $P_{\text{co}}(\cdot, \sigma, \sigma_{\text{co}})$ has a unique minimiser S_h for any $0 < h < h_0$ and arbitrary $0 < \sigma < \beta_1$ and $0 < \sigma_{\text{co}} < \beta_{\text{co}}$. This minimiser satisfies for $s_h = T_M S_h$ the relation

$$\mathcal{E}_M(s_h) \leq \mathcal{E}_M(f^*) + c h^\alpha \|f^*\|_{H^2(M)}^2$$

with $\alpha = \min\{\sigma/2, \beta_2/2, \beta_1 - \sigma, \beta_{\text{co}} - \sigma_{\text{co}}\}$. For the approximation of the constraints it holds

$$A_M^{\text{co}}(s_h - g_{\text{co}}) \leq c h^{\sigma_{\text{co}}} \|f^*\|_{H^2(M)}^2.$$

Proof: We write as before \mathcal{E}_T for the formulation of \mathcal{E}_M in terms of derivatives in tangent directions. Because there is no need to distinguish the exact decomposition of \mathcal{E} into its total and augmentary portions, nor to distinguish between an intrinsic and a tangent directional version of A_M^{co} , we just write A in the following for the sake of readability, and we state that as usual an uppercase argument of A is to be considered in the trace sense on M . Then again by the optimality of S_h we obtain due to the fact that $f^* \in D_{\text{co}}$, with $\vec{F}^* = E_N f^*$ in the respective trace or point evaluation sense, the relation

$$\begin{aligned} & \mathcal{E}_T(S_h) + h^{-\sigma} N_M^\nabla(S_h) + h^{-\sigma} N_C^\nabla(S_h) + h^{-\sigma_{\text{co}}} A(S_h - \vec{F}^*) \\ & \leq \mathcal{E}_T(S_h^*) + h^{-\sigma} N_M^\nabla(S_h^*) + h^{-\sigma} N_C^\nabla(S_h^*) + h^{-\sigma_{\text{co}}} A(S_h^* - \vec{F}^*). \end{aligned} \quad (5.7.1)$$

As before in (5.5.2) we deduce that $N_M^\nabla(S_h^*) \leq c h^{\beta_1} \|f^*\|_{H^2(M)}^2$ and

$$\mathcal{E}_T(S_h^*) \leq \mathcal{E}_M(\vec{S}_h^*) + c \sqrt{\mathcal{E}_M(\vec{S}_h^*)} \sqrt{N_M^\nabla(S_h^*)} + c N_M^\nabla(S_h^*). \quad (5.7.2)$$

We further conclude by insertion of these into (5.7.1) that

$$\mathcal{E}_T(S_h) + h^{-\sigma} N_M^\nabla(S_h) + h^{-\sigma} N_C^\nabla(S_h) + h^{-\sigma_\infty} A(S_h - \vec{F}^*) \leq c \|f^*\|_{H^e(M)}^2.$$

So consequently

$$\begin{aligned} A(S_h - \vec{F}^*) &\leq c h^{\sigma_\infty} \|f^*\|_{H^e(M)}^2 \\ N_M^\nabla(S_h) &\leq c h^\sigma \|f^*\|_{H^e(M)}^2 \\ \mathcal{E}_T(S_h) &\leq c \|f^*\|_{H^e(M)}^2. \end{aligned}$$

We conclude as before thanks to positivity of both sides in (5.7.1) by insertion of our recent findings the relation

$$\begin{aligned} \mathcal{E}_T(S_h) &\leq \mathcal{E}_T(S_h^*) + h^{-\sigma} N_M^\nabla(S_h^*) + h^{-\sigma} N_C^\nabla(S_h^*) + h^{-\sigma_\infty} A(S_h - \vec{F}^*) \\ &\leq \mathcal{E}_M(S_h^*) + c (h^{\beta_1/2} + h^{\beta_1 - \sigma} + h^{\beta_\infty - \sigma_\infty}) \|f^*\|_{H^e(M)}^2. \end{aligned}$$

As before in the derivation of (5.5.3) and (5.5.4) we obtain

$$\mathcal{E}_M(S_h) \leq \mathcal{E}_T(S_h) + c \sqrt{\mathcal{E}_M(S_h)} \cdot h^{\sigma/2} \|f^*\|_{H^e(M)}$$

and conclude like for (5.5.5) that indeed

$$\mathcal{E}_M(S_h) \leq \mathcal{E}_M(S_h^*) + c (h^{\sigma/2} + h^{\beta_1 - \sigma} + h^{\beta_\infty - \sigma_\infty}) \|f^*\|_{H^e(M)}^2. \quad (5.7.3)$$

Because of the triangle inequality in $L_2(\Gamma_\ell)$ or Euclidean space, we have that

$$c h^{\beta_\infty/2} \|f^*\|_{H^e(M)} \geq \sqrt{A(S_h^* - \vec{F}^*)} \geq \left| \sqrt{A(S_h^*)} - \sqrt{A(\vec{F}^*)} \right|.$$

We obtain by Jensen's inequality $\|\cdot\|_1^2 \leq c_1 \|\cdot\|_2^2 \leq c_2 \|\cdot\|_1^2$ and because the sum of $A(\cdot)$ and $\mathcal{E}_M(\cdot)$ is elliptic on $H^2(M)$ that $\sqrt{\mathcal{E}_M(\cdot)} + \sqrt{A(\cdot)}$ is an equivalent norm on $H^2(M)$. So we can deduce by norm equivalence and the inverse triangle inequality

$$\left| \sqrt{\mathcal{E}_M(S_h^*)} - \sqrt{\mathcal{E}_M(\vec{F}^*)} + \sqrt{A(S_h^*)} - \sqrt{A(\vec{F}^*)} \right| \leq c \|s_h^* - f^*\|_{H^2(M)} \leq c h^{\beta_2/2} \|f^*\|_{H^e(M)}.$$

Making use of the inverse triangle inequality therein, we see by continuity of \mathcal{E}_M that

$$\begin{aligned} \left| \sqrt{\mathcal{E}_M(S_h^*)} - \sqrt{\mathcal{E}_M(\vec{F}^*)} \right| &\leq c \|s_h^* - f^*\|_{H^2(M)} + \left| \sqrt{A(S_h^*)} - \sqrt{A(\vec{F}^*)} \right| \\ &\leq c (h^{\beta_2/2} + h^{\beta_\infty/2}) \|f^*\|_{H^e(M)} \leq c h^{\beta_2/2} \|f^*\|_{H^e(M)}. \end{aligned}$$

By continuity of \mathcal{E}_M we can furthermore deduce that

$$\sqrt{\mathcal{E}_M(S_h^*)} + \sqrt{\mathcal{E}_M(\vec{F}^*)} \leq c \|f^*\|_{H^e(M)}.$$

Consequently again the third binomial gives that

$$|\mathcal{E}_M(S_h^*) - \mathcal{E}_M(\vec{F}^*)| \leq c h^{\beta_2/2} \|f^*\|_{H^\varrho(M)}^2,$$

whereby in particular

$$\mathcal{E}_M(S_h^*) \leq \mathcal{E}_M(\vec{F}^*) + c h^{\beta_2/2} \|f^*\|_{H^\varrho(M)}^2.$$

This gives directly by insertion into (5.7.3) that

$$\mathcal{E}_M(S_h) - \mathcal{E}_M(\vec{F}^*) \leq c (h^{\beta_2/2} + h^{\sigma/2} + h^{\sigma-\beta_1} + h^{\beta_{\text{co}}-\sigma_{\text{co}}}) \|f^*\|_{H^\varrho(M)}^2.$$

The claimed relation follows then by addition of $\mathcal{E}_M(\vec{F}^*)$ on both sides. \square

5.8 Remark: (1) Note that although we have lost the absolute value in the bound, the worst thing that can happen is that the energy of s_h is *below* the energy of the optimal solution in D_{co} due to some additional freedom left by the penalty when compared to strict conditions.

(2) Note also that while our prime objective is the case of finite Ξ , the above arguments remain valid also for example if Γ is a curve in a surface, or even if it is a subsurface, provided the conditions on the combined functionals are satisfied — so we could thereby even demand that the solution vanishes on a subdomain of M .

(3) Note further again that $\beta_{\text{co}} \geq \beta_2$ is guaranteed by continuity of the embedding $H^2(M) \hookrightarrow L_2(\Gamma_\ell)$ due to the trace theorem, or by the embedding $H^2(M) \hookrightarrow C(M)$ required in case of nonempty Ξ , but better values may be achievable.

5.3 Penalty Approximation for Energy Residuals

In contrast to the previous section, we can achieve a remarkable improvement in the theoretical convergence rates for our APA minimisation if we have a residual in the functional arguments, so $\mathcal{E}(f - f_0)$ for fixed $f_0 \in H^\varrho(M)$ as we have encountered it when we introduced and discussed the "PDE functional" $\mathcal{E}_\Delta^\lambda$ in Theorem 4.54. Generalising this approach now, we demand that we have an augmented E_N -extrinsic functional $\mathcal{E}_M \in \mathbb{E}_N^g(M)$ without linear part, and that we are given $f_0 \in H^\varrho(M)$ or from some convex subset D_{co} of that space. Then we consider $\mathcal{E}_M(f - f_0)$ and obtain thereby a kind of "shifted" functional, whose obvious minimum is attained in $f = f_0$. We can then formulate a suitable penalty functional

$$P_{f_0}(S, \sigma) = P(S - E_N f_0, \sigma),$$

once we note that we can omit $-E_N f_0$ in N_M^∇, N_C^∇ of $P_{f_0}(S, \sigma)$, as it vanishes in both of them by conception.

In case we include the constraints that specify D_{co} into the functional in the form $\mathcal{E}_M + A_M^{co}$ and wish to enforce $A_M^{co}(f - f_0) \rightarrow 0$ further, we also obtain a modified version

$$P_{f_0}(S, \sigma, \sigma_{co}) = \mathcal{E}_T(S - E_N f_0) + h^{-\sigma_{co}} A_M^{co}(S - E_N f_0) + h^{-\sigma} N_M^\nabla(S) + h^{-\sigma} N_C^\nabla(S).$$

In the following, we choose the latter approach as the more general one, keeping in mind that we can always choose $\sigma_{co} = 0$ to end up in the first version, and we deduce the following result:

5.9 Theorem *Let $M \in \mathbb{M}_{bd}^k(\mathbb{R}^d)$ and let $D_{co} \subseteq H^2(M)$ be a closed, convex set, characterised by $A_M^{co}(f - g_0) = 0$ for fixed $g_0 \in H^2(M)$ and augmentary E_N -extrinsic functional A_M^{co} . Let \mathcal{E}_M be a bilinear E_N -extrinsic functional on $H^2(M)$ such that $\mathcal{E}_M^{co} = \mathcal{E}_M + A_M^{co} \in \mathbb{E}_N^s(M)$ is elliptic. Let $f_0 \in D_{co}$ be arbitrary. Let $(s_h^*)_{h < h_0}$ be a family of restrictions of approximations $(S_h^*)_{h < h_0} \in \text{App}(f_0, \varrho, \beta_1, \beta_2)$ to $\overline{F}_0 = E_N f_0$ such that for some suitable $\beta_{co} \geq \beta_2$ and any $0 < h < h_0$ additionally*

$$A_M^{co}(s_h^* - f_0) \leq c h^{\beta_{co}} \|f_0\|_{H^e(M)}^2.$$

Then $P_{f_0}(\cdot, \sigma, \sigma_{co})$ has a unique minimiser S_h for any $0 < h < h_0$ and arbitrary $0 < \sigma < \beta_1$ and $0 \leq \sigma_{co} < \beta_{co}$. This minimiser satisfies for $s_h = T_M S_h$ the relation

$$\|s_h - f_0\|_{H^2(M)}^2 \leq c h^\alpha \|f_0\|_{H^e(M)}^2$$

with $\alpha = \min\{(\beta_1 + \beta_2)/2, \beta_2, \beta_1 - \sigma, \beta_{co} - \sigma_{co}\}$. For the approximation of the augmentary constraints it holds further

$$A_M^{co}(s_h - f_0) \leq c h^{\alpha + \sigma_{co}} \|f_0\|_{H^e(M)}^2.$$

Proof: We write as usual \mathcal{E}_T for the formulation of \mathcal{E}_M in terms of derivatives in tangent directions. As before, we obtain then

$$\begin{aligned} N_M^\nabla(S_h^*) &\leq c h^{\beta_1} \|f_0\|_{H^e(M)}^2 \\ N_C^\nabla(S_h^*) &\leq c h^{\beta_1} \|f_0\|_{H^e(M)}^2 \\ A_M^{co}(s_h^* - f_0) &\leq c h^{\beta_{co}} \|f_0\|_{H^e(M)}^2. \end{aligned}$$

With these bounds we deduce like in (5.5.2) from the convergence orders provided by the hypotheses that thanks to continuity and bilinearity of \mathcal{E}_M

$$\begin{aligned}\epsilon_T(S_h^* - \vec{F}_0) &\leq \epsilon_M(\vec{S}_h^* - \vec{F}_0) + c \sqrt{\epsilon_M(\vec{S}_h^* - \vec{F}_0)} \sqrt{N_M^\nabla(S_h^*)} + c N_M^\nabla(S_h^*) \\ &\leq c (h^{\beta_2} + h^{\beta_2/2+\beta_1/2} + h^{\beta_1}) \cdot \|f_0\|_{H^e(M)}^2.\end{aligned}$$

Consequently, we obtain for $\alpha = \min\{(\beta_1 + \beta_2)/2, \beta_2, \beta_1 - \sigma, \beta_{co} - \sigma_{co}\}$ by insertion into the relation $P_{f_0}(S_h, \sigma, \sigma_{co}) \leq P_{f_0}(S_h^*, \sigma, \sigma_{co})$ that

$$\epsilon_T(S_h - \vec{F}_0) + h^{-\sigma} N_M^\nabla(S_h) + h^{-\sigma} N_C^\nabla(S_h) + h^{-\sigma_{co}} A_M^{co}(S_h - f_0) \leq c h^\alpha \cdot \|f_0\|_{H^e(M)}^2.$$

So in particular $N_M^\nabla(S_h) \leq c h^{\alpha+\sigma} \|f_0\|_{H^e(M)}^2$ and furthermore

$$\epsilon_T(S_h - \vec{F}_0) \leq c h^\alpha \|f_0\|_{H^e(M)}^2 \quad \text{and} \quad A_T^{co}(S_h - \vec{F}_0) \leq c h^{\alpha+\sigma_{co}} \|f_0\|_{H^e(M)}^2. \quad (5.9.1)$$

Investigating $\epsilon_T(S_h - \vec{F}_0)$ further, we see, similar to deducing (5.5.3), that it holds

$$\begin{aligned}\epsilon_T(S_h - \vec{F}_0) &\geq \epsilon_M(S_h - \vec{F}_0) - c \sqrt{\epsilon_M(S_h - \vec{F}_0)} \sqrt{N_M^\nabla(S_h)} \\ &\geq \epsilon_M(S_h - \vec{F}_0) - c \sqrt{\epsilon_M(S_h - \vec{F}_0)} \cdot h^{(\alpha+\sigma)/2} \|f_0\|_{H^e(M)}.\end{aligned}$$

This gives us with some necessary but simple restructurings like those performed to deduce (5.5.4) that

$$\begin{aligned}\epsilon_M(S_h - \vec{F}_0) &\leq \epsilon_T(S_h - \vec{F}_0) + c \sqrt{\epsilon_M(S_h - \vec{F}_0)} \cdot h^{(\alpha+\sigma)/2} \|f_0\|_{H^e(M)} \\ &\leq c h^\alpha \cdot \|f_0\|_{H^e(M)}^2 + c \sqrt{\epsilon_M(S_h - \vec{F}_0)} \cdot h^{(\alpha+\sigma)/2} \|f_0\|_{H^e(M)}.\end{aligned} \quad (5.9.2)$$

If we now solve the quadratic equation as in the previous proofs, we can even deduce that

$$\sqrt{\epsilon_M(S_h - \vec{F}_0)} \leq c \cdot \left(h^{\alpha/2+\sigma/2} \|f_0\|_{H^e(M)} \pm \sqrt{h^{\alpha+\sigma} \|f_0\|_{H^e(M)}^2 + 4h^\alpha \|f_0\|_{H^e(M)}^2} \right),$$

so in particular $\sqrt{\epsilon_M(S_h - \vec{F}_0)} \leq c h^{\alpha/2} \|f_0\|_{H^e(M)}$. We insert this into (5.9.2) to conclude that

$$\epsilon_M(S_h - \vec{F}_0) \leq c h^\alpha \cdot \|f_0\|_{H^e(M)}^2 + c h^{\alpha/2} \cdot h^{\alpha/2+\sigma/2} \|f_0\|_{H^e(M)}^2 \leq c h^\alpha \cdot \|f_0\|_{H^e(M)}^2.$$

Turning now to the side condition treatment, we know already by the second relation in (5.9.1) that $A_M^{co}(S_h - \vec{F}_0) \leq c h^{\sigma_{co}+\alpha} \|f_0\|_{H^e(M)}^2$. This yields the desired result, as we consequently obtain for elliptic $\epsilon_M^{co} = \epsilon_M + A_M^{co}$ that

$$\|s_h - f_0\|_{H^2(M)}^2 \leq c \cdot \epsilon_M^{co}(s_h - f_0) = c \cdot \epsilon_M(s_h - f_0) + c \cdot A_M^{co}(s_h - f_0) \leq c h^\alpha \|f_0\|_{H^e(M)}^2.$$

□

5.10 Remark: (1) Both $\mathcal{E}_\Delta^\lambda$ and \mathcal{E}_Δ^Ξ (with a single point constraint) fall under the assumptions of this result on ESMs without boundary. We will later investigate these in further detail.

(2) Note again that a value of $\beta_{\text{co}} = \beta_2$ is always guaranteed by continuity of the embedding $H^2(\mathcal{M}) \hookrightarrow L_2(\Gamma_\ell)$ or $H^2(\mathcal{M}) \hookrightarrow C(\mathcal{M})$ in case of nonempty Ξ . However, better values may be achievable depending on the respective specific choice of the functional and the regularity of its minimiser.

(3) Note further that the impact of σ on the rate of convergence is significantly lower than in the previous theorems: raising σ has no positive impact anymore, and even $\sigma = 0$ is a valid choice. In fact, *any* choice of σ with $\alpha \geq \beta_1 - \sigma$ is valid and has no relevant impact on the convergence rate — a fact we found also confirmed in practice, although there still is an impact on stability.

It should also be noted that ellipticity of $\mathcal{E}_\mathcal{M} + A_\mathcal{M}^{\text{co}}$ was only relevant at the very end of the proof, and effectively anything achieved before this point remains valid also for mere augmented $E_\mathcal{N}$ -extrinsic functionals; only, we may run into problems with the unique solvability. If this is ensured by whatever other arguments, we can rescue most of the previous result. To achieve this unique solvability in practice, it suffices to have that $\mathcal{E}_\mathcal{M}$ is positive definite on any $S_h^m(C_h(\mathcal{M}))$ or the respective superset $S_h^m(\widehat{C}_h(\mathcal{M}))$ that is actually considered.

5.11 Corollary *Let $\mathcal{M} \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ and let $\mathcal{E}_\mathcal{M} = B_\mathcal{M} + A_\mathcal{M} \in \mathbb{E}_\mathcal{N}^\Xi(\mathcal{M})$ be an augmented, positive semidefinite $E_\mathcal{N}$ -extrinsic functional on $H^2(\mathcal{M})$ such that $\mathcal{E}_\mathcal{M} + A_\mathcal{M}^{\text{co}}$ is positive definite on any $S_h^m(C_h(\mathcal{M}))$ for $0 < h < h_0$, and let $\mathcal{E}_\mathcal{T}, B_\mathcal{T}, A_\mathcal{T}, A_\mathcal{T}^{\text{co}}$ be the corresponding tangent Euclidean derivative formulations. Let $f_0 \in H^\varrho(\mathcal{M})$ be arbitrary but fixed. Let $(s_h^*)_{h < h_0}$ be a family of restrictions of approximations $(S_h^*)_{h < h_0} \in \text{App}(f_0, \varrho, \beta_1, \beta_2)$ to $\overline{F} = E_\mathcal{N} f_0$ such that for some suitable $\beta_{\text{co}} \geq \beta_2$ and any $0 < h < h_0$ additionally*

$$A_\mathcal{M}(s_h^* - f_0) \leq c h^{\beta_{\text{co}}} \|f_0\|_{H^\varrho(\mathcal{M})}^2.$$

Then $P_{f_0}(\cdot, \sigma, \sigma_{\text{co}})$ has a unique minimiser S_h for any $0 < h < h_0$ and arbitrary $0 < \sigma < \beta_1$ and $0 \leq \sigma_{\text{co}} < \beta_{\text{co}}$. This minimiser satisfies for $s_h = \mathcal{T}_\mathcal{M} S_h$ the relation

$$\|s_h - f_0\|_{H^2(\mathcal{M})}^2 \leq c h^\alpha \|f_0\|_{H^\varrho(\mathcal{M})}^2$$

with $\alpha = \min\{(\beta_1 + \beta_2)/2, \beta_2, \beta_1 - \sigma, \beta_{\text{co}} - \sigma_{\text{co}}\}$. For the approximation of the augmented constraints it holds further

$$A_\mathcal{M}(s_h - f_0) \leq c h^{\alpha + \sigma_{\text{co}}} \|f_0\|_{H^\varrho(\mathcal{M})}^2.$$

The relevance of this corollary can be exemplified by the partial differential equation $\Delta_M f = g$ on some M_0 under homogeneous Dirichlet boundary conditions for nonempty boundary Γ_0 . The positive semidefiniteness of the corresponding functional is obvious, and the definiteness on finite dimensional subspaces of the space $C^2(\text{clos}(M_0))$ is also easily seen: Any function in the kernel would have to be harmonic, and the only harmonic function under zero boundary conditions is the zero function. To see this, note that by Green's theorem any function $f \in C^2(M_0)$ that solves the homogeneous equation will also satisfy

$$0 = - \int_{M_0} f \cdot \Delta_M f = \int_{M_0} \langle \nabla_M f, \nabla_M f \rangle,$$

which clearly implies $f = 0$ by continuity, regardless of the question of ellipticity or coercivity of the functional on all of $H^2(M_0)$. Similarly, we can also apply this to the more general case of an equation of the form $\Delta_M f - \lambda f = g$ under Dirichlet conditions, as we have again that any function in the kernel of the corresponding functional must vanish on the boundary and therefore satisfy

$$\begin{aligned} 0 &= \int_{M_0} (\Delta_M f - \lambda f)^2 = \int_{M_0} (\Delta_M f)^2 - 2\lambda \int_{M_0} f \Delta_M f + \int_{M_0} (\lambda f)^2 \\ &= \int_{M_0} (\Delta_M f)^2 + 2\lambda \int_{M_0} \langle \nabla_M f, \nabla_M f \rangle - 0 + \int_{M_0} (\lambda f)^2, \end{aligned}$$

which clearly implies $f = 0$ also for $\lambda > 0$. In the same fashion, other suitable equations and conditions can be handled, provided appropriate formulations as E_N -extrinsic functionals are available.

5.4 Penalty Approximation of Energies with Linear Portion

If ultimately the augmented E_N -extrinsic functional $\mathcal{E}_M = B_M + \Lambda_M + A_M$ is given with nonvanishing $\Lambda_M \in \mathbb{L}_M(A_M, B_M)$ subordinate to $B_M + A_M$, then none of the previous results will apply. Indeed the situation is far more difficult now, as there is a considerable linear part Λ_M in \mathcal{E}_M we have to deal with.

However, by conception of Λ_M we can suppose that there is some "common ground" for any functional value. That is, we have $\varepsilon_\Lambda \geq 0$ such that *simultaneously* $\mathcal{E}_M(\cdot) + \varepsilon_\Lambda \geq 0$ and $\mathcal{E}_T(\cdot) + \varepsilon_\Lambda \geq 0$, as we have demanded it in the definition of augmented equivalently E_N -extrinsic energy functionals with nonvanishing linear part. Then we define a suitable penalty functional as before for elliptic $\mathcal{E}_M^\pi = B_M + A_M$ and corresponding $\mathcal{E}_T^\pi = B_T + A_T$ as

$$P_\Lambda(S, \sigma) := \mathcal{E}_T(S) + h^{-\sigma} N_M^\nabla(S) + h^{-\sigma} N_C^\nabla(S).$$

Now we can also state and prove a convergence result for this type of functional and generalise Theorem 5.5 in that respect:

5.12 Theorem *Let $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ and let $\mathcal{E}_M = B_M + A_M + \Lambda_M \in \mathbb{E}_N(M)$ be an augmented functional on $H^2(M)$ for elliptic $\mathcal{E}_M^\alpha = B_M + A_M$. Let $\varepsilon_\Lambda \geq 0$ be chosen such that $\mathcal{E}_M(\cdot) + \varepsilon_\Lambda \geq 0$ and $\mathcal{E}_T(\cdot) + \varepsilon_\Lambda \geq 0$. Let $f^* \in H^e(M)$ be the unique minimiser of \mathcal{E}_M . Let $(s_h^*)_{h < h_0}$ be a family of restrictions of approximations $(S_h^*)_{h < h_0} \in \text{App}(f^*, \varrho, \beta_1, \beta_2)$. Then $P_\Lambda(\cdot, \sigma)$ has a unique minimiser S_h for any $0 < h < h_0$ and arbitrary $0 < \sigma < \beta_1$. The trace $s_h = T_M S_h$ of this minimiser satisfies the relation*

$$\|s_h - f^*\|_{H^2(M)} \leq c h^\alpha \mathcal{E}_\Lambda^*(f),$$

where $\alpha := \min\{\beta_1/2, \beta_2/2, \beta_1 - \sigma, \sigma/2\}$ and $\mathcal{E}_\Lambda^*(f) = \mathcal{E}_\Lambda(f) + \sqrt{\mathcal{E}_\Lambda(f)}$ for

$$\mathcal{E}_\Lambda(f) = \|f^*\|_{H^e(M)}^2 + \|f^*\|_{H^e(M)} + \varepsilon_\Lambda.$$

Again, all statements remain valid in a closed convex subset D_{co} of $H^2(M)$ as long as $(S_h^*)_{h < h_0}$ and $(S_h)_{h < h_0}$ are also obtained from D_{co} .

Proof: As usual, we denote by $\mathcal{E}_T = \mathcal{E}_T^\alpha + \Lambda_T$ the corresponding formulation of $\mathcal{E}_M = \mathcal{E}_M^\alpha + \Lambda_M$ in terms of derivatives in tangent directions. We can clearly bound as usual by optimality of S_h

$$\mathcal{E}_T(S_h) + h^{-\sigma} N_M^\nabla(S_h) + h^{-\sigma} N_C^\nabla(S_h) \leq \mathcal{E}_T(S_h^*) + h^{-\sigma} N_M^\nabla(S_h^*) + h^{-\sigma} N_C^\nabla(S_h^*). \quad (5.12.1)$$

As before we obtain that it holds

$$N_M^\nabla(S_h^*) \leq c h^{\beta_1} \|f^*\|_{H^e(M)}^2 \quad \text{and} \quad N_C^\nabla(S_h^*) \leq c h^{\beta_1} \|f^*\|_{H^e(M)}^2$$

and that by Conclusion 4.67 similar to (5.5.2)

$$\begin{aligned} \mathcal{E}_T^\alpha(S_h^*) &= \mathcal{E}_T^\alpha(S_h^* - \vec{S}_h^* + \vec{S}_h^*) \\ &= \mathcal{E}_T^\alpha(\vec{S}_h^*) + \mathcal{E}_T^\alpha(S_h^* - \vec{S}_h^*) + 2\mathcal{E}_T^\alpha(S_h^* - \vec{S}_h^*, \vec{S}_h^*) \\ &\leq \mathcal{E}_T^\alpha(\vec{S}_h^*) + c \sqrt{\mathcal{E}_T^\alpha(\vec{S}_h^*)} \sqrt{N_M^\nabla(S_h^*)} + c N_M^\nabla(S_h^*) \\ &\leq \mathcal{E}_T^\alpha(\vec{S}_h^*) + c \sqrt{\mathcal{E}_T^\alpha(\vec{S}_h^*)} \sqrt{h^{\beta_1} \|f^*\|_{H^e(M)}^2} + c h^{\beta_1} \|f^*\|_{H^e(M)}^2. \end{aligned}$$

At the same time we have that

$$\begin{aligned} \mathcal{E}_T^\alpha(\vec{S}_h^*) &= \mathcal{E}_M^\alpha(s_h^*) = \mathcal{E}_M^\alpha(s_h^* - f^* + f^*) = \mathcal{E}_M^\alpha(s_h^* - f^*) + \mathcal{E}_M^\alpha(f^*) + 2\mathcal{E}_M^\alpha(s_h^* - f^*, f^*) \\ &\leq \mathcal{E}_M^\alpha(f^*) + c \|s_h^* - f^*\|_{H^2(M)}^2 + c \|s_h^* - f^*\|_{H^2(M)} \|f^*\|_{H^2(M)} \end{aligned}$$

$$\leq \mathcal{E}_M^\alpha(f^*) + c h^{\beta_2} \|f^*\|_{H^e(M)}^2 + c h^{\beta_2/2} \|f^*\|_{H^e(M)}^2 \leq \mathcal{E}_M^\alpha(f^*) + c h^{\beta_2/2} \|f^*\|_{H^e(M)}^2$$

and thus in particular $\mathcal{E}_T^\alpha(\vec{S}_h^*) \leq c \|f^*\|_{H^e(M)}^2$. Thereby we have also that

$$\begin{aligned} \mathcal{E}_T^\alpha(S_h^*) &\leq \mathcal{E}_M^\alpha(f^*) + c (h^{\beta_1/2} + h^{\beta_2/2}) \|f^*\|_{H^e(M)}^2 \\ &\leq c (1 + h^{\beta_1/2} + h^{\beta_2/2}) \|f^*\|_{H^e(M)}^2. \end{aligned} \quad (5.12.2)$$

Regarding the linear portion, we obtain with Conclusion 4.69 that

$$\begin{aligned} \Lambda_T(S_h^*) &= \Lambda_T(\vec{S}_h^*) + \Lambda_T(S_h^* - \vec{S}_h^*) \leq \Lambda_M(s_h^*) + c h^{\beta_1/2} \|f^*\|_{H^e(M)} \\ &\leq \Lambda_M(f^*) + |\Lambda_M(s_h^* - f^*)| + c h^{\beta_1/2} \|f^*\|_{H^e(M)} \\ &\leq \Lambda_M(f^*) + c h^{\beta_2/2} \|f^*\|_{H^e(M)} + c h^{\beta_1/2} \|f^*\|_{H^e(M)} \end{aligned} \quad (5.12.3)$$

$$\leq \|f^*\|_{H^e(M)} + c h^{\beta_2/2} \|f^*\|_{H^e(M)} + c h^{\beta_1/2} \|f^*\|_{H^e(M)}. \quad (5.12.4)$$

Inserting (5.12.2) and (5.12.4) in (5.12.1) we obtain

$$\begin{aligned} &\mathcal{E}_T^\alpha(S_h) + \Lambda_T(S_h) + h^{-\sigma} N_M^\nabla(S_h) + h^{-\sigma} N_C^\nabla(S_h) \\ &\leq c (1 + h^{\beta_1/2} + h^{\beta_2/2} + h^{\beta_1-\sigma}) \|f^*\|_{H^e(M)}^2 + c (1 + h^{\beta_1/2} + h^{\beta_2/2}) \|f^*\|_{H^e(M)} \\ &\leq c (1 + h^{\beta_1/2} + h^{\beta_2/2} + h^{\beta_1-\sigma}) \mathcal{E}_\Lambda(f). \end{aligned} \quad (5.12.5)$$

We add ε_Λ on both sides now, and then we deduce from the positivity we have achieved thereby that in particular

$$N_M^\nabla(S_h) \leq c h^\sigma \mathcal{E}_\Lambda(f), \quad N_C^\nabla(S_h) \leq c h^\sigma \mathcal{E}_\Lambda(f).$$

From this we can deduce similar to the previous situations, in particular when obtaining (5.5.3), that with Conclusions 4.67, 4.68 and 4.69 and ellipticity of \mathcal{E}_M^α it holds

$$\begin{aligned} \mathcal{E}_T^\alpha(S_h) + \Lambda_T(S_h) &= \mathcal{E}_T^\alpha(S_h - \vec{S}_h + \vec{S}_h) + \Lambda_T(S_h - \vec{S}_h + \vec{S}_h) \\ &= \mathcal{E}_T^\alpha(\vec{S}_h) + \mathcal{E}_T^\alpha(S_h - \vec{S}_h) + 2\mathcal{E}_T^\alpha(S_h - \vec{S}_h, \vec{S}_h) + \Lambda_T(S_h - \vec{S}_h) + \Lambda_T(\vec{S}_h) \\ &\geq \mathcal{E}_T^\alpha(\vec{S}_h) + \Lambda_T(\vec{S}_h) - \mathcal{E}_T^\alpha(S_h - \vec{S}_h) - 2|\mathcal{E}_T^\alpha(S_h - \vec{S}_h, \vec{S}_h)| - |\Lambda_T(S_h - \vec{S}_h)| \\ &\geq \mathcal{E}_M^\alpha(s_h) + \Lambda_M(s_h) - c (1 + \sqrt{\mathcal{E}_M^\alpha(s_h)}) \cdot h^{\sigma/2} (\mathcal{E}_\Lambda(f))^{\frac{1}{2}}. \end{aligned}$$

This gives us for $\mathcal{E}_M^+(\cdot) := \mathcal{E}_M(\cdot) + \varepsilon_\Lambda \geq 0$ and corresponding $\mathcal{E}_T^+(\cdot) := \mathcal{E}_T(\cdot) + \varepsilon_\Lambda \geq 0$

$$\mathcal{E}_M^+(s_h) \leq \mathcal{E}_T^+(S_h) + c (1 + \sqrt{\mathcal{E}_M^\alpha(s_h)}) \cdot h^{\sigma/2} (\mathcal{E}_\Lambda(f))^{\frac{1}{2}}. \quad (5.12.6)$$

Positivity of $\mathcal{E}_T^+(S_h)$ gives us then via (5.12.5) that

$$\mathcal{E}_M^+(s_h) \leq c \mathcal{E}_\Lambda^*(s_h) + c (1 + \sqrt{\mathcal{E}_M^\sharp(s_h)}) h^{\sigma/2} \mathcal{E}_\Lambda^*(f). \quad (5.12.7)$$

What we need now is that for a constant c independent of s_h

$$1 + \sqrt{\mathcal{E}_M^\sharp(s_h)} \leq c \sqrt{\mathcal{E}_M^+(s_h)}. \quad (5.12.8)$$

By continuity of Λ_M and ellipticity of \mathcal{E}_M^\sharp it holds in particular that for a constant c_e that depends only on \mathcal{E}_M^\sharp and Λ_M (and thus on \mathcal{E}) that

$$\mathcal{E}_M^+(s_h) = \mathcal{E}_M^\sharp(s_h) + \Lambda_M(s_h) + \varepsilon_\Lambda \geq \mathcal{E}_M^\sharp(s_h) - c_e \sqrt{\mathcal{E}_M^\sharp(s_h)} + \varepsilon_\Lambda.$$

Without restriction we can demand that $\varepsilon_\Lambda \geq 1$ and $c_e \geq 2$, as both values are not bounded from above by any requirements. Then it suffices for (5.12.8) to prove that for suitable $c > 0$

$$\mathcal{E}_M^\sharp(s_h) + c_e \sqrt{\mathcal{E}_M^\sharp(s_h)} + \varepsilon_\Lambda \leq c (\mathcal{E}_M^\sharp(s_h) - c_e \sqrt{\mathcal{E}_M^\sharp(s_h)} + \varepsilon_\Lambda). \quad (5.12.9)$$

To prove that, it is obviously sufficient to prove the relation for $c = 2$. Then (5.12.9) reduces to a comparably simple relation for univariate quadratic functions: We just need to find out whether any $t \in [0, \infty[$ satisfies $t^2 + c_e t + \varepsilon_\Lambda \leq 2(t^2 - c_e t + \varepsilon_\Lambda)$, which can be transformed into

$$0 \leq 2t^2 - 2c_e t + 2\varepsilon_\Lambda - t^2 - c_e t - \varepsilon_\Lambda = t^2 - 3c_e t + \varepsilon_\Lambda. \quad (5.12.10)$$

It can then directly be seen that the map

$$t \mapsto t^2 - 3c_e t + \varepsilon_\Lambda$$

is increasing in $[\frac{2}{3}c_e, \infty[$, so it suffices to prove that (5.12.10) is valid in $[0, \frac{2}{3}c_e[$. To achieve this, we further suppose without restriction that $\varepsilon_\Lambda \geq 2c_e^2$. This means no harm as we can choose ε_Λ arbitrarily large, as long this choice is fixed for specific Λ_M . Then it holds $\varepsilon_\Lambda - 3c_e t \geq 2c_e^2 - 3c_e t \geq 2c_e^2 - 2c_e^2 = 0$. This gives (5.12.9) and thus (5.12.8). So we can deduce from (5.12.7) that in particular

$$\mathcal{E}_M^+(s_h) \leq c (1 + h^{\sigma/2} \sqrt{\mathcal{E}_M^+(s_h)}) \mathcal{E}_\Lambda^*(f).$$

We conclude again from the corresponding quadratic equation that

$$\mathcal{E}_M^+(s_h) \leq c \mathcal{E}_\Lambda^*(f). \quad (5.12.11)$$

We use this to obtain from (5.12.6) the inequality

$$\mathcal{E}_M^+(s_h) \leq \mathcal{E}_T^+(S_h) + c h^{\sigma/2} \mathcal{E}_\Lambda^*(f). \quad (5.12.12)$$

Then we combine our findings to deduce that

$$\begin{aligned} \mathcal{E}_M^\alpha(f^*) + \Lambda_M(f^*) + \varepsilon_\Lambda &\leq \mathcal{E}_M^\alpha(s_h) + \Lambda_M(s_h) + \varepsilon_\Lambda \leq \mathcal{E}_T^\alpha(S_h) + \Lambda_T(S_h) + \varepsilon_\Lambda + c h^{\sigma/2} \mathcal{E}_\Lambda^*(f) \\ &\leq \mathcal{E}_T^\alpha(S_h) + \Lambda_T(S_h) + \varepsilon_\Lambda + h^{-\sigma} N_M^\nabla(S_h) + h^{-\sigma} N_C^\nabla(S_h) + c h^{\sigma/2} \mathcal{E}_\Lambda^*(f) \\ &\leq \mathcal{E}_T^\alpha(S_h^*) + \Lambda_T(S_h^*) + \varepsilon_\Lambda + h^{-\sigma} N_M^\nabla(S_h^*) + h^{-\sigma} N_C^\nabla(S_h^*) + c h^{\sigma/2} \mathcal{E}_\Lambda^*(f) \\ &\leq \mathcal{E}_M^\alpha(f^*) + \Lambda_M(f^*) + \varepsilon_\Lambda + c (h^{\beta_1/2} + h^{\beta_2/2} + h^{\beta_1 - \sigma} + h^{\frac{\sigma}{2}}) \mathcal{E}_\Lambda^*(f), \end{aligned}$$

where we used in particular the optimality of f^* in the first inequality, (5.12.12) in the second, (5.12.1) in the fourth and (5.12.2), (5.12.3) in the fifth relation. Thereby we can draw the conclusion that

$$\mathcal{E}_M^\alpha(f^*) + \Lambda_M(f^*) \leq \mathcal{E}_M^\alpha(s_h) + \Lambda_M(s_h) \leq \mathcal{E}_M^\alpha(f^*) + \Lambda_M(f^*) + c h^\alpha \mathcal{E}_\Lambda^*(f),$$

where we define $\alpha := \min\{\beta_1/2, \beta_2/2, \beta_1 - \sigma, \sigma/2\}$. This yields now indeed convergence of functional values to the optimum in the form

$$|\mathcal{E}_M(s_h) - \mathcal{E}_M(f^*)| \leq c h^\alpha \mathcal{E}_\Lambda^*(f).$$

By Conclusion 4.56 we deduce convergence of functions. □

Chapter 6

Scattered Data Problems on Embedded Submanifolds

In this chapter, we are going to investigate certain approximation problems based on a finite set of scattered data sites Ξ sampled from an ESM $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$. We will look for applications of ambient penalty approximation of the minima to some of the specific energy functionals introduced before. These approximate solutions will be based on tensor product splines.

We will not focus on the standard situation in scattered data approximation problems, where one demands that the sites Ξ are rather well-sampled and more or less uniformly distributed over M , and that function values in the sites are reliable and effectively exact. Instead, we will concentrate on the more complex situations where one faces some lack in the data, either introduced by sparsity, noisy function values or nonuniform distribution, with data sites that are dense in some but sparse in other areas of M .

6.1 Sparse Data Extrapolation

Our first objective is the problem of extrapolation from a comparably sparse set Ξ of data sites: There are comparably few data sites, and intricate geometric features in between of them that need to be resolved. We demand therein that we are given some corresponding set of function values Y . The task is to determine “reasonable” function values for the rest of M based on the given values in the sites, and in particular to resolve the geometric features of the ESM in order to make our approximation as independent of these features as possible. We begin our discussion with a short revision of comparably standard approaches, and why the presence of sparsity — or the lack of data — introduces additional difficulties that implies the need for a new approach.

6.1.1 Problem Statement and Naive Approaches

Just the problem of interpolation in an arbitrary set Ξ of scattered data sites in \mathbb{R}^d itself is a nontrivial matter. As the scattering makes some standard approaches like (higher order) polynomials or (to some degree) even splines hardly applicable, one would often rely on the so-called *meshless methods* therein (cf. [17, 40, 105]). Two of the perhaps most prominent examples of these are *moving least squares* and *radial basis functions*. Both of these are capable of providing pleasant convergence behaviour once the data gets denser and denser in terms of a decrease of the *fill distance*

$$h_{\Xi, \Omega} = \sup_{x \in \Omega} \min_{\xi \in \Xi} \|x - \xi\|_2.$$

And even if the data is sparse, there are special cases of these methods that are capable of producing highly satisfactory results in \mathbb{R}^d : For example, in terms of moving least squares, one can rely on the very basic concept of *inverse distance weighting*, i.e. moving least squares of order one. There, one simply determines the extrapolation function as

$$u_{\Xi, Y}(x) = \sum_{\xi \in \Xi} v_{\xi} \frac{u(\|x - \xi\|_2)}{\sum_{\zeta \in \Xi} u(\|x - \zeta\|_2)}$$

for an appropriate weight function $u(\cdot)$ that is related to the inverse distance of the two arguments (cf. [46, 48, 53, 70, 92, 105]). For radial basis functions, there are in particular the celebrated polyharmonic splines or thin-plate splines. These are defined as $\mathbb{P}_{d,m}(x, \xi) = b_{d,m}(\|x - \xi\|_2)^{(1)}$ with

$$b_{d,m}(t) = \begin{cases} t^{2m-d} & d \text{ odd} \\ t^{2m-d} \log(t) & d \text{ even} \end{cases}$$

and depend on the respective dimension d and naturally require $m > d/2$. They yield, under the assumption of sufficient polynomial unisolvency (cf. [105]), an interpolant of the form

$$\sum_{\xi \in \Xi} \alpha_{\xi} \mathbb{P}_{d,m}(x, \xi) + P_m(x),$$

for a suitable polynomial $P_m \in \mathcal{P}^m(\mathbb{R}^d)$ and suitable coefficients $\alpha_{\xi} \in \mathbb{R}$ (cf. [105]). The resulting interpolant will then even minimise the Euclidean version of the Hessian energy under interpolation constraints over all of \mathbb{R}^d in case $m = 2$ (cf. [105]).

If we turn to the submanifold setting, we can obtain a solution to an interpolation

⁽¹⁾We use the nonstandard letters “ \mathbb{P}, \mathfrak{p} ” in $\mathbb{P}_{d,m}, b_{d,m}$ instead of the usual $\Phi_{d,m}, \phi_{d,m}$ to avoid confusion with the compactly supported Wendland functions that are usually also abbreviated $\Phi_{d,m}, \phi_{d,m}$. These letters are the greek letters “Sho” to express a “sh”, and simultaneously the norse letters “Thorn” that represent a “th” like in the “thin” of *thin-plate spline*.

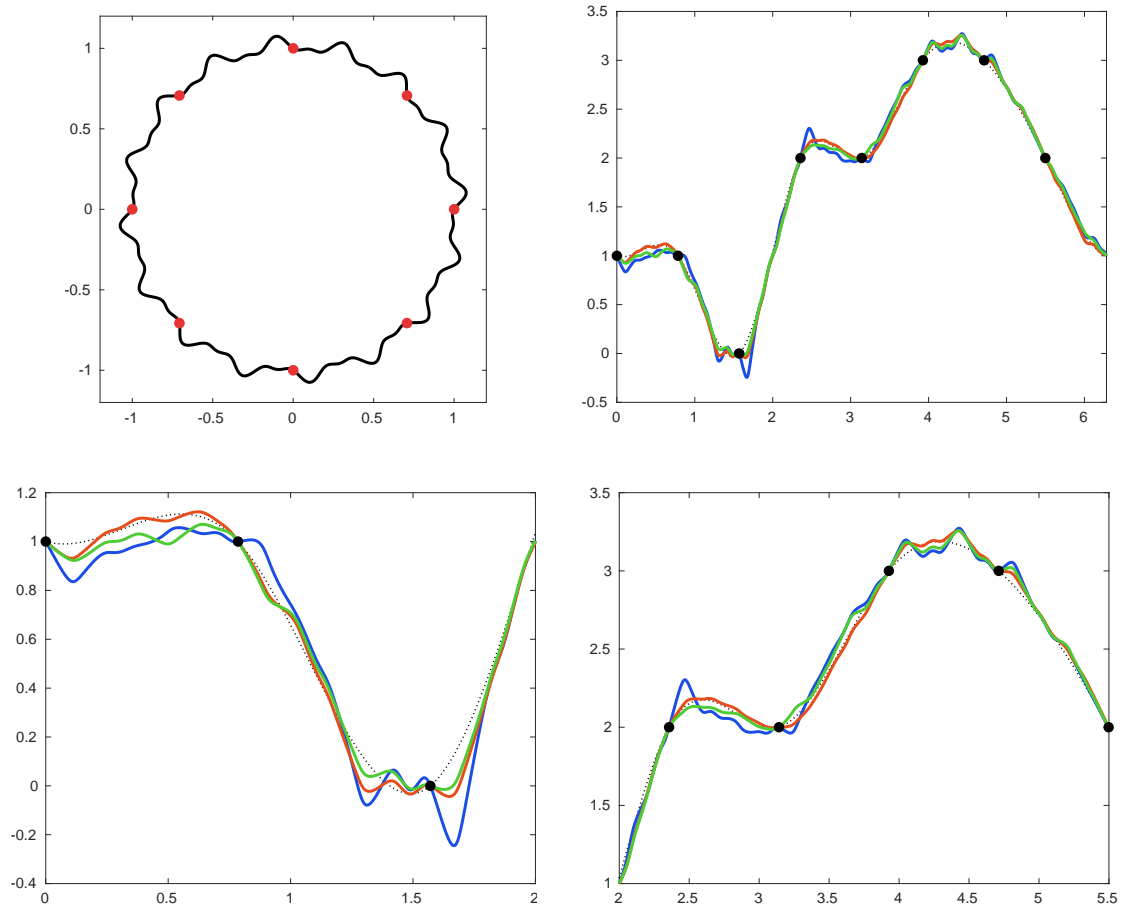


Figure 6.1: Results of naive approach to extrapolation: Top left depicted is a closed curve with intricate geometry and some data sites on it. Top right is the plot of restrictions of different direct interpolations to function values 1, 1, 0, 2, 2, 3, 3, 2, assigned counterclockwise with starting from point (1, 0) along the curve. Depicted is an arc-length proportional evaluation for the “standard interval” $[0, 2\pi]$ we use here and always in future for closed curves. Black dotted: “Benchmark” of a suitable extrapolation, based on univariate periodic cubic splines. Blue: Linear triangulated spline interpolation based on a Delaunay triangulation of the points (cf. [6], as provided by Matlab®). Orange: Interpolation for Wendland function $\phi_{3,1}$ and support radius 10.0 (cf. [105, Ch. 9]). Green: Interpolation for polyharmonic spline $p_{2,2}$. Bottom left, bottom right: Close-ups of the results that emphasise the artifacts.

problem on M by solving it in \mathbb{R}^d with one of the presented methods and restricting the solution. In case of RBF, this simple restriction of the solution to M will yield a reasonable approximation as soon as the intrinsic version of the fill distance

$$h_{\Xi, M} = \sup_{x \in M} \min_{\xi \in \Xi} d_M(x, \xi)$$

is sufficiently small (cf. [49]). However, the problem of any approach where the approximation is determined from the data sites without considering the underlying ESM is that it will become increasingly unreliable when the data gets sparser. In that case, the problem can no longer be considered as if the points were part of a

linear subspace locally, which is the case when the data is sufficiently dense. Now the geometry of the ESM between the data sites becomes increasingly relevant and can introduce undesirable artifacts (see Fig. 6.1).

6.1 Remark: (1) What can be said about approximation on ESMs in general does of course hold in a sparse data setting in particular: Direct intrinsic function spaces will hardly be available in a reasonable way — so aside from sphere, torus and the like, we cannot hope for any intrinsic space to solve our extrapolation problem, and chart-based methods might even be exposed to a case where a couple of charts contain no data at all.

(2) Inverse distance weighting could of course also be employed with the intrinsic geodesic distance d_M instead of the Euclidean distance of the ambient space, and thereby generalise to M without facing the danger of geometry-induced artifacts. But then one would have to consider only ESMs where calculation of the distance is possible for any two points, so effectively it would need to be complete. And even if we have that, the calculation of the distance to any point in Ξ would be required for any evaluation of the extrapolation, whereby the whole approach can become very costly.

6.1.2 Extrapolation by Penalty Based Energy Minimisation

Now that we have clarified the need for a method to extrapolate suitably on a subdomain $M_0 \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ of an ESM $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$, we can turn to provide one. Luckily, we have actually everything prepared to accomplish this already: We just need to consider the energies \mathcal{E}_H^Ξ or on compact ESMs also \mathcal{E}_Δ^Ξ for a D_M^2 -unisolvent, finite set $\Xi \in M_0$, and insert them in the APA minimisations of Section 5.2. Thereby we obtain, with $M \in \mathbb{M}_{\text{cp}}^k(\mathbb{R}^d)$ in case of the Laplacian energy, the APA functionals

$$\begin{aligned} P_{H,M_0}(S, \sigma_M, \sigma_C) &:= \mathcal{E}_H^T(S) + h^{-\sigma_M} N_M^\nabla(S, M_0) + h^{-\sigma_C} N_C^\nabla(S, M_0), \\ P_{\Delta,M}(S, \sigma_M, \sigma_C) &:= \mathcal{E}_\Delta^T(S) + h^{-\sigma_M} N_M^\nabla(S, M) + h^{-\sigma_C} N_C^\nabla(S, M), \end{aligned}$$

where we understand $\mathcal{E}_H^T, \mathcal{E}_\Delta^T$ as the tangent versions of $\mathcal{E}_H, \mathcal{E}_\Delta$ and suppose the desired function values in Ξ to be given by $Y_\Xi = \{\gamma_\xi\}_{\xi \in \Xi}$. Therein, S is a linear combination of the tensor product B-splines that is active on the set $C_h(M_0)$. Any such S is further required a priori to satisfy the interpolation constraints strictly here. The respective versions with the constraints included as a penalty are then

$$\begin{aligned} P_{H,M_0}^\Xi(S, \sigma_M, \sigma_C, \sigma_\Xi) &:= P_{H,M_0}(S, \sigma_M, \sigma_C) + h^{-\sigma_\Xi} \sum_{\xi \in \Xi} (S(\xi) - \gamma_\xi)^2, \\ P_{\Delta,M}^\Xi(S, \sigma_M, \sigma_C, \sigma_\Xi) &:= P_{\Delta,M}(S, \sigma_M, \sigma_C) + h^{-\sigma_\Xi} \sum_{\xi \in \Xi} (S(\xi) - \gamma_\xi)^2. \end{aligned}$$

In practice, we will usually replace $C_h(M_0)$ by suitable supersets, like the set of all cells whose center has distance at most h to M_0 . This does not affect the solvability and other relevant properties of the method, as we have stated in the beginning of the previous chapter.

In the rest of this section we are going to investigate the effect of these functionals further. Therein, we put our focus on the first two and use fixed interpolation constraints. This is done because we are investigating convergence orders in practice, and thus at least at some point we will have enough degrees of freedom to solve the problem reasonably under the strict constraints.

In all examples below, we demand that the ESM was initially smooth, but is now just represented by a large number of small connected triangles (or line segments in the case of curves) and corresponding normals in the vertices. This is sufficient for the method, with the integration performed by the linear approximation that the triangles (or line segments) allows us to do.

Having in mind future applications for real life data where only such a representation is available (like the "triangle soup" commonly provided even for smooth surfaces by the .stl, .cgr data formats or the like) this seemed to be appropriate, while for the sake of comparability and reasonable error measurement, we restrict ourselves here to artificially determined data that is a sort of "downsampled" from smooth ESMs.

6.2 Remark: We should briefly address the problem of approximate integration on ESMs further, which is inevitable in our situation. As announced, we chose the "brute force" approach of simple piecewise linear approximate integration based on the discretisation of the (initially smooth) ESM by triangles (or line segments) we have — effectively, we could even go for Riemannian sums, if we have only a dense point cloud with associated normals. Of course, one could also go for far more elaborate solutions to the problem, but it should be kept in mind that we hope to get away with far less degrees of freedom in the spline space than we have triangle vertices — and even a Riemannian sum over several hundreds of thousands of points is more or less appropriate when you have just a few thousand B-splines. And even better, as the integration over $C_h(M_0)$ is not contributing to the quality of the process and the approximation results except in terms of stability of the linear systems, we can use this very basic approach also for the integration on the cells.

We now turn to a short analysis of what we can expect by this approach before we finally come to the examples; we first would like to investigate convergence and the choice of the penalty exponents σ_M , σ_C and σ_Ξ . Unfortunately, the optimal solution is only known explicitly if M is a curve (closed or open), where the optimum is the periodic or natural cubic spline, assigned by an arc-length parameterisation. For

the more interesting case of surfaces, the explicit optimal solution is unknown if it is not constant, and therefore we have no optimum to compare with. So we can only exemplify the results of the method in the surface case for various examples to verify that the results are still reasonable.

In the curve case, the regularity of the optimal solution is at least $H^{3.5-\varepsilon}$, and we can apply the results on ambient approximation methods for $H^2(\mathbb{M})$ and for normal derivatives to obtain suitable values for α in Theorem 5.5: By Corollary 3.33 we can expect that there is a family $(s_h^*)_{h < h_0}$ of restrictions of splines $(S_h^*)_{h < h_0}$ such that

$$\|s_h^* - f^*\|_{H^2(\mathbb{M})}^2 \leq c h^{2(1.5-\varepsilon)} \|f^*\|_{H^{3.5}(\mathbb{M})}^2$$

and thus we deduce that $\beta_2 \approx 3$, and by Corollary 3.39 we can expect from the same family that

$$\|T_{\mathbb{M}}(\nabla_N S_h^*)\|_{L_2(\mathbb{M})}^2 \leq c h^{2(2.5-\varepsilon)} \|f^*\|_{H^{3.5}(\mathbb{M})}^2$$

and therefore we deduce $\beta_1 \approx 5$. So we have a family of splines $(S_h^*)_{h < h_0}$ that is approximately in $\text{App}(f^*, 3.5, 5, 3)$, and can apply Theorem 5.5 on approximation by APA minimisation in convex sets. Thus we conclude that we can expect at least convergence of order $\alpha/2$ in $H^2(\mathbb{M})$ for $\alpha = \min\{\sigma/2, 3/2, 5 - \sigma\}$. Thereby, it seems that the optimal choice for σ is $10/3$, if we set $\sigma_{\mathbb{M}} = \sigma_{\mathbb{C}}$ as in our theoretical results. But the best choice from a practical point of view is actually lower. This seems to have at least two reasons:

1. Apparently, any choice of about $\sigma \geq 2$ seems to imply convergence of order at least $h^{3/2}$ in practice.
2. The use of $\sigma = 3$ can lead to numerical dominance of the penalty part quite rapidly, whereby saturation effects can occur faster and with stronger impact.

It can further be beneficial to the practical results (in absolute terms, not in terms of orders) if one uses a "space penalty exponent" $\sigma_{\mathbb{C}}$ lower than the "ESM penalty exponent" $\sigma_{\mathbb{M}}$. The reason for this seems to be that the space penalty consumes a considerable amount of approximation power if stressed too much, while it does actually not contribute to the convergence behaviour substantially — it is only there to stabilise the system. In Fig. 6.2 we have depicted convergence orders for the initial example of Fig. 6.1, "ESM penalties" h^{-2}, h^{-3} and "space penalties" h^{-1}, h^{-2}, h^{-3} , and for the same function values and arc-length relations between points on the unit circle. Roughly speaking, the choices $\sigma_{\mathbb{C}} = 2, \sigma_{\mathbb{M}} = 2$, $\sigma_{\mathbb{C}} = 1, \sigma_{\mathbb{M}} = 3$ and $\sigma_{\mathbb{C}} = 2, \sigma_{\mathbb{M}} = 3$ seem to give comparable results, whereas the two extremal choices

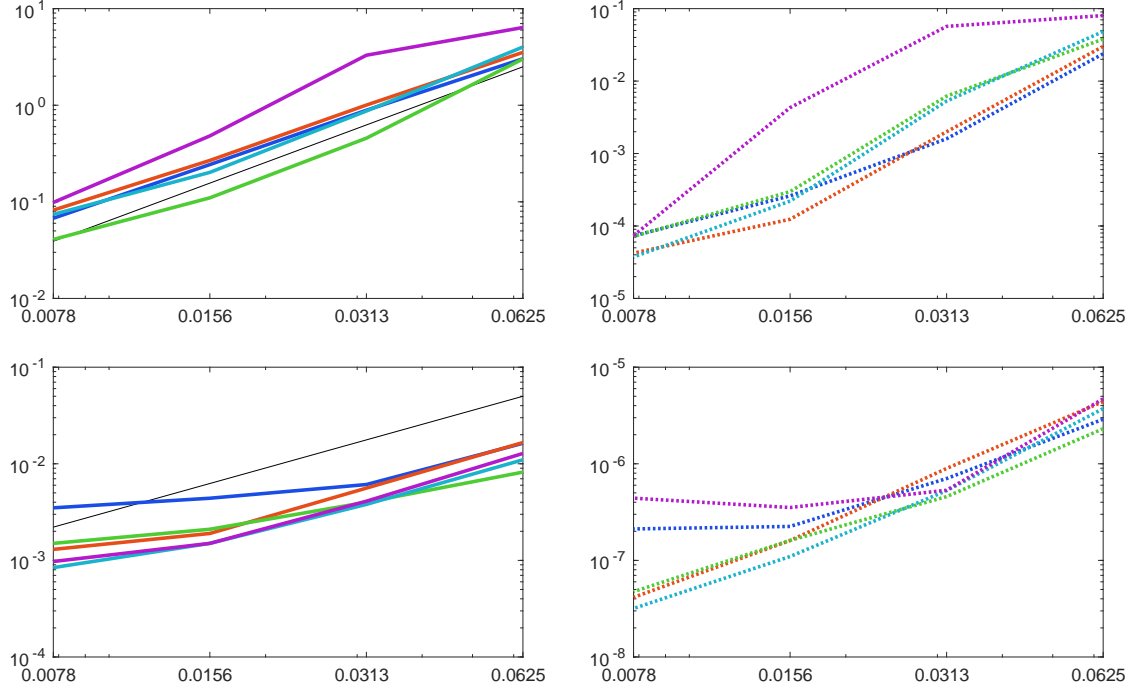


Figure 6.2: Results of penalty energy approximations to problem of Fig. 6.1 in the upper row (with reference h^2) and to the unit circle in the lower row (with reference $h^{3/2}$). Blue: $\sigma_C = 1, \sigma_M = 2$. Orange: $\sigma_C = 2, \sigma_M = 2$. Green: $\sigma_C = 1, \sigma_M = 3$. Cyan: $\sigma_C = 2, \sigma_M = 3$. Purple: $\sigma_C = 3, \sigma_M = 3$. Solid lines for energy rms, dotted for L_2 -rms.

provide some disadvantages in one or the other situation. In our tests below, we will present results for $\sigma_C = 2, \sigma_M = 2$ and $\sigma_C = 2, \sigma_M = 3$.

6.3 Remark: (1) We also see that we can effectively restrict ourselves to cubic splines, so order $m = 4$: all other choices would not give a higher order of convergence, and because of their favorable ratio of cell and support sizes, cubics are the most stable and most local choice one can make here (recall that we have required C^2 functions, so minimally $m = 4$).

(2) Exponents σ_M significantly smaller than 2 turn out to provide inferior results both with respect to actual results and convergence rates. In particular, $\sigma_M = 1$ would multiply the error by roughly 10 and reduce the rate of convergence by half.

6.4 Remark: (1) As stated elsewhere, we do not only use those cells active on the ESM for the “space penalty”, but all cells whose center has distance to the ESM less than h . This surely includes all cells active on the ESM in our cases of $d = 2, 3$ and is easier to check than actual intersection. In particular, the danger of “missing” a relevant cell because of slight inaccuracies in the intersection test is clearly reduced thereby. On the other hand, it does surely no harm to the convergence, provided we also use all the B-Splines active on these cells in our method.

(2) In the implementation, we did not care about the validity of the closest point property. Instead, for any point in space considered, we simply took the closest

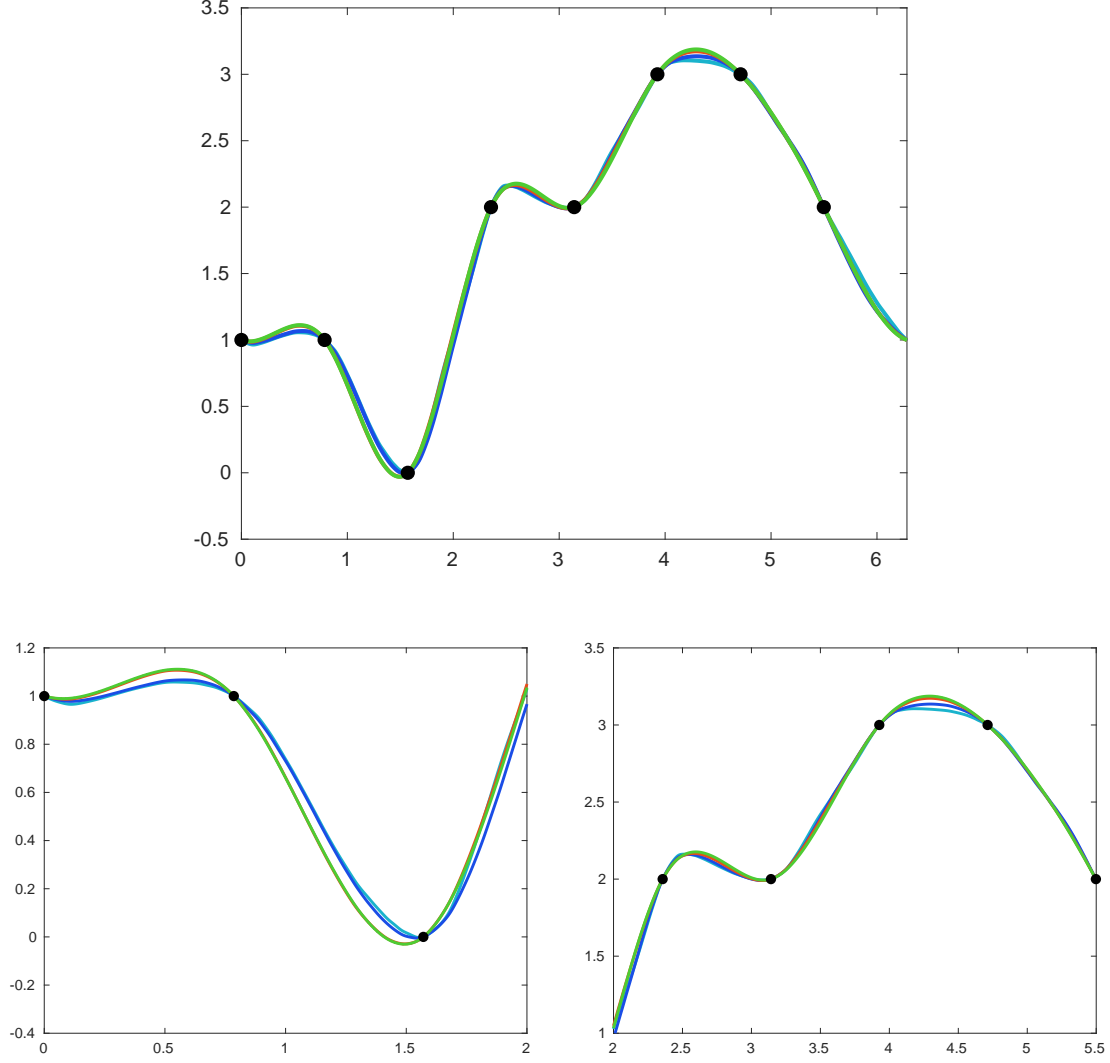


Figure 6.3: Results of penalty energy approximations to problem of Fig. 6.1 for cell widths $h = 0.08$ (cyan), $h_1 = 0.06$ (blue), $h_2 = 0.04$ (orange), $h_3 = 0.02$ (green) with additional close-up. Although the “goal” of a cubic is also depicted theoretically, it cannot be distinguished anymore from the green curve. Again, anything is presented as obtained by arc-length proportional parameterisation on “standard interval” $[0, 2\pi]$. The penalty exponent was chosen as $\sigma = 2$.

point in the discretisation of the ESM, although this is theoretically not necessarily unique. However, the results were nonetheless more than satisfactory, as we can see in Fig. 6.3. This implies that the approach is rather robust towards inaccuracies in the projection.

In order to provide some practical convergence analysis, we will now consider in addition to the initial example all the curves and functions presented in Fig. 6.4 and Fig. 6.5. There, we present curves with both comparably smooth and rather intricate geometries, for equally and inequally spaced data sites, open and closed curves and in particular also for one choice of sites that yields an intrinsic version of a linear polynomial, so an optimal solution $f^* \in C^\infty(M)$.

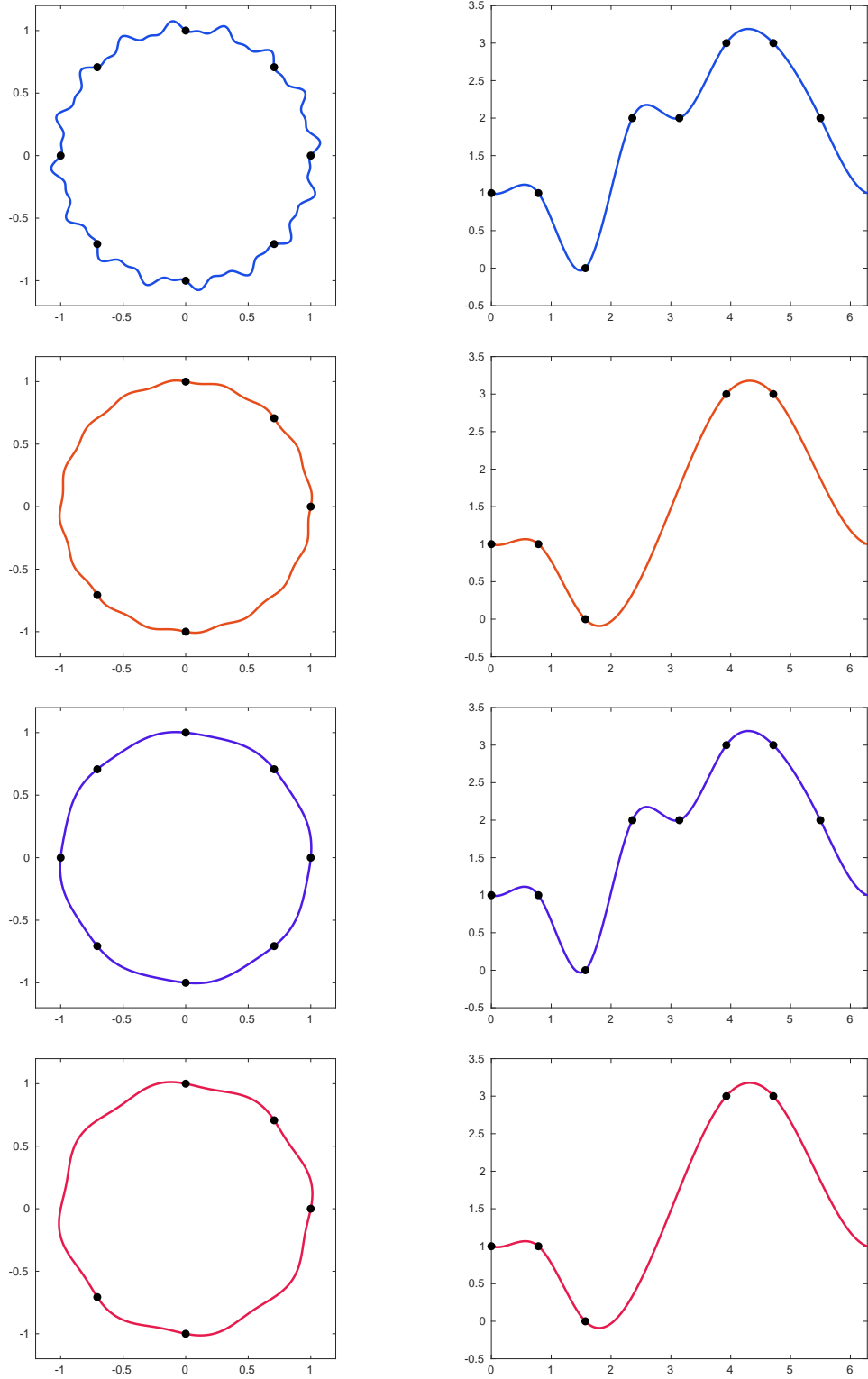


Figure 6.4: First column: Closed curves used for testing, with data sites depicted. Function values for closed curve, starting from site $(1, 0)$ counter-clockwise: $1, 1, 0, 2, 2, 3, 3, 2$ for the first and third curve, and $1, 1, 0, 3, 3$ for the second and fourth. Second column: Plot of respective optimal solutions, depicted as arc-length proportional “unrolled” functions on our standard interval $[0, 2\pi]$. Convergence plots are presented in Fig. 6.6.

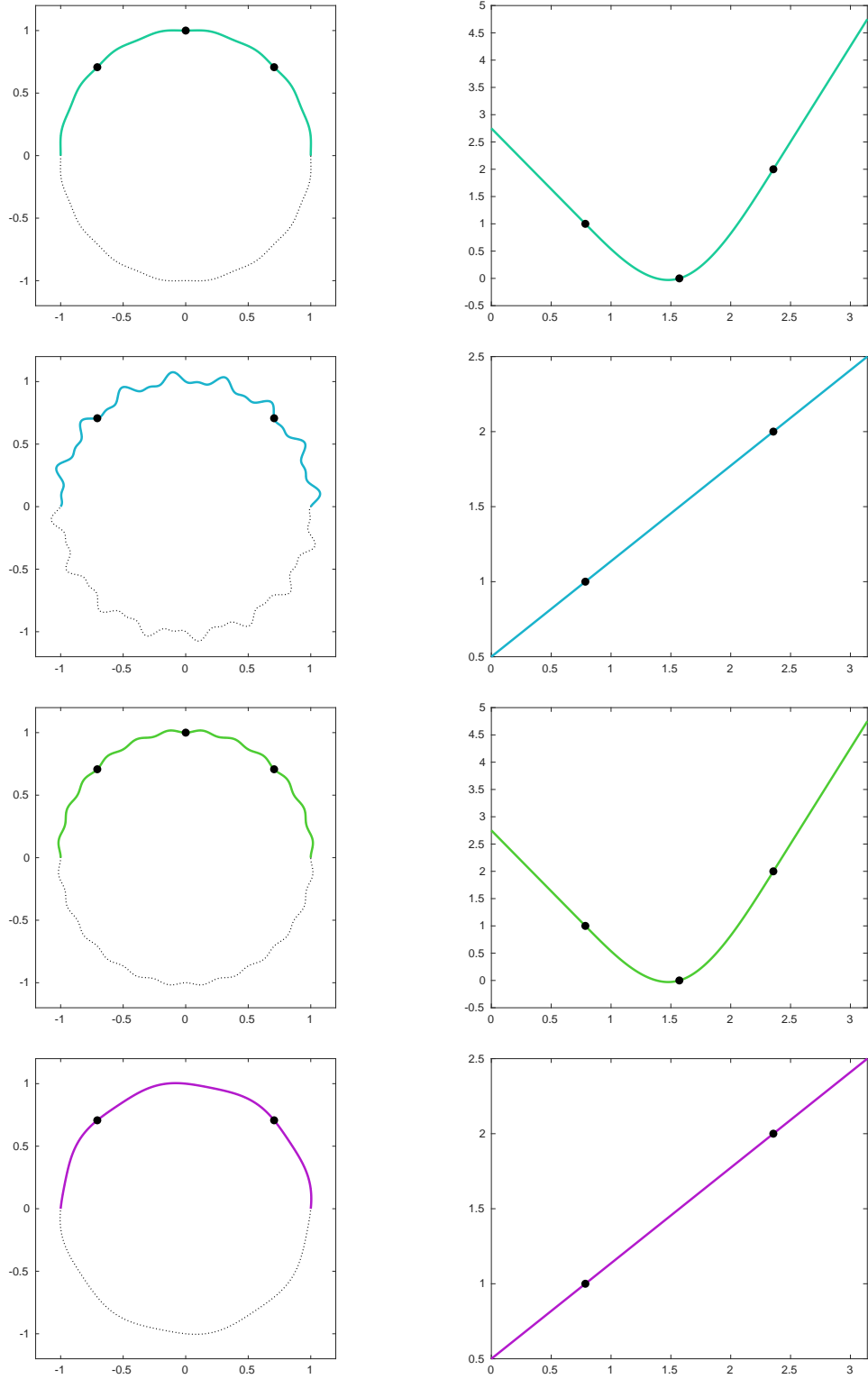


Figure 6.5: First column: Open curves used for testing, with data sites depicted. Pictures contain also (dotted) the closure that was used in a small region around boundary points for determining the projections. Function values for closed curve, starting from site $(1, 0)$ counter-clockwise: 1, 0, 2 for the first and third, and 1, 2 for the second and forth curve. Second column: Plot of respective optimal solutions, depicted as arc-length proportional "unrolled" functions on our standard interval $[0, \pi]$. Convergence plots are presented in Fig. 6.6.

The observed order of convergence in Fig. 6.6 in the energy norm (L_2 -norm of the second derivative) is surprisingly high: Roughly speaking, it is effectively rather h^2 than the expected value of about $h^{3/4}$. Several possible explanations seem conceivable, in particular

- The division by 2 for σ and β_2 that occurs in determining convergence exponent α from Theorem 5.5 is actually unnecessary, and the theoretical convergence is nearly optimal also in the present case.
- The normal derivatives decay faster than expected by the penalty: In all cases, we have essentially a decay by a factor of at least h^2 or even about h^3 instead

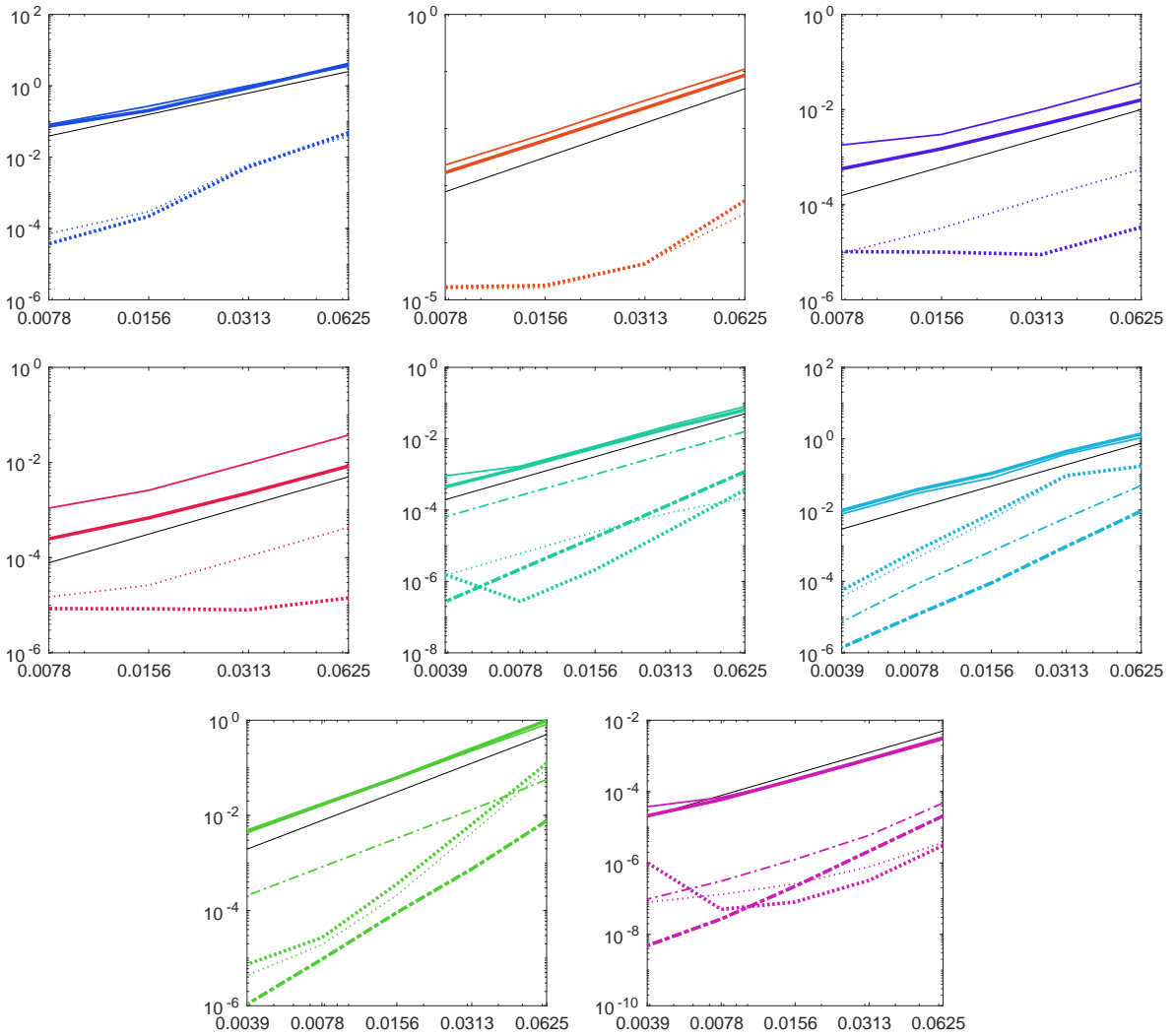


Figure 6.6: Convergence orders for examples presented in Fig. 6.4 (first quadruple of plots) and Fig. 6.5 (second quadruple of plots), colors reference the respective curves and functions: — energy error (colored: approximation, black: reference h^2), L_2 error (colored: approximation) for about $600[1/h]$ points (closed curves) and about $300[1/h]$ (open curves) points, - - - normal derivative (colored: approximation). The thicker lines are for $\sigma_C = 2, \sigma_M = 3$, the thinner lines for $\sigma_C = 2, \sigma_M = 2$.

of the expected h^1 , depending on the penalty exponent. This can lead to a change in the convergence behaviour because of the faster approximation of "intrinsic energy" by "extrinsic energy". However, as the errors in normal directions (depicted dash-dotted) are by orders of magnitude smaller than those for the energy, and the decrease for $\sigma_M = 3$ has no effect on the energy error, this seems rather unlikely.

- The exact regularity of the solution is possibly higher than the $H^{3.5-\varepsilon}(M_0)$ available in determining β_2 : we may have even $H^{4-\delta}(M_0)$ for some small value $\delta > 0$.
- The regularity, and therefore the convergence, is further increased by constant extension for this specific function, which itself does not feature singularities but only breaks in the higher order derivatives. This cannot be covered by our convergence analysis up to now, but might improve the convergence behaviour further.

On the other hand, the convergence behaviour of the L_2 error is not so easy to describe, and it does not show such a clear convergence behaviour. Apparently, it is still roughly controlled by the energy error, but the actual behaviour can (for example in the green and cyan curve examples) but must not be better than that. And it seems to reach a saturation at about $10^{-5} - 10^{-8}$, so at least several orders of magnitude less than the saturation of the energy. As mentioned before, the saturation that occurs in particular for $\sigma_M = 3$ might be introduced by numerical dominance of the penalised part of the functional, particularly for $\sigma_M = 3$: For $h = 2^{-8}$ as in the last step of the convergence analysis, this means a penalty of $2^{24} \approx 16.78$ millions.

Now we turn to practical examples on surfaces. As we have no analytical optimum directly at hand here, we will just present examples that prove the validity of our approach. This time, we will also for the first time distinguish between energy based on Laplacian and on Hessian, but it will turn out that there is not so much difference when the outcome is concerned.

Inspired by the previous examples for curves, we consider a comparable surface, roughly resembling a pumpkin and depicted in Fig. 6.7. It is obtained for $\theta_{12}(x, y) = 12 \tan_2^{-1}(x, y)$ as the level-1-surface of function

$$(x, y, z) \mapsto \left(x \left(1 - \frac{(1 - z^2)^2 \sin(\theta_{12}(x, y))}{20} \right) \right)^2 + \left(y \left(1 - \frac{(1 - z^2)^2 \sin(\theta_{12}(x, y))}{20} \right) \right)^2 + z^2.$$

Note in particular that the surface is rotation symmetric for rotation around the z -axis by multiples of $\pi/2$, but it is not reflection symmetric to the (x, z) -plane or (y, z) -plane.

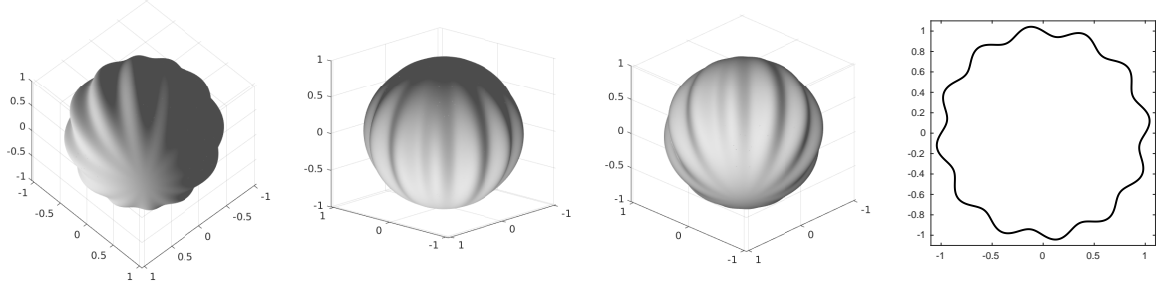


Figure 6.7: Left: 3d-representation of the "pumpkin" from several viewpoints. Right: The equator of the "pumpkin", so its section with the (x, y) -plane.

This pumpkin is sampled in about 165'000 points and 330'000 triangles. We handle it with cells of length $h = 0.1$, which means that about 9'000 B-splines are employed. Thereby, we show that we can achieve satisfactory results even with comparably large h ; as we have no direct information on the regularity of the optimum f^* , we use the penalty exponent $\sigma = 2$ for both σ_M and σ_C , because we found this to give good results in the previous case, and it is less demanding in terms of the regularity and approximation order than $\sigma_M = 3$.

6.5 Remark: When the data is obtained from a smooth implicit function as in the case of the pumpkin, then it can be reasonable to use the gradient flow to determine the directional derivatives in the ambient space — instead of the normal of the closest point. By this choice, the problem of projection is circumvented; as the resulting extension operator is still orthogonal we loose nothing on the approximation power even in theory. Such implicit representation can be obtained even for point clouds by suitable approximation methods as proposed in [40, Ch. 30], if normals in the points can be provided or extrapolated and no implicit function is given already.

But let us now turn to the first examples. We impose function values that make us expect a function that is symmetric to the (x, z) -plane or (y, z) -plane, but not rotation symmetric, and so we can verify that indeed the geometry of the ESM is outruled. We demand function values given by assigning on the one hand

$$(1, 0, 0) \mapsto 1, (0, 1, 0) \mapsto 1, (-1, 0, 0) \mapsto 1, (0, -1, 0) \mapsto 1, (0, 0, 1) \mapsto 0, (0, 0, -1) \mapsto 0$$

and on the other hand

$$(1, 0, 0) \mapsto 1, (0, 1, 0) \mapsto 0, (-1, 0, 0) \mapsto -1, (0, -1, 0) \mapsto 0, (0, 0, 1) \mapsto 0, (0, 0, -1) \mapsto 0$$

on the pumpkin. The results are depicted in Fig. 6.8. There, we see results for both "Hessian" and "Laplacian" energy in APA extrapolation, and we find that there is

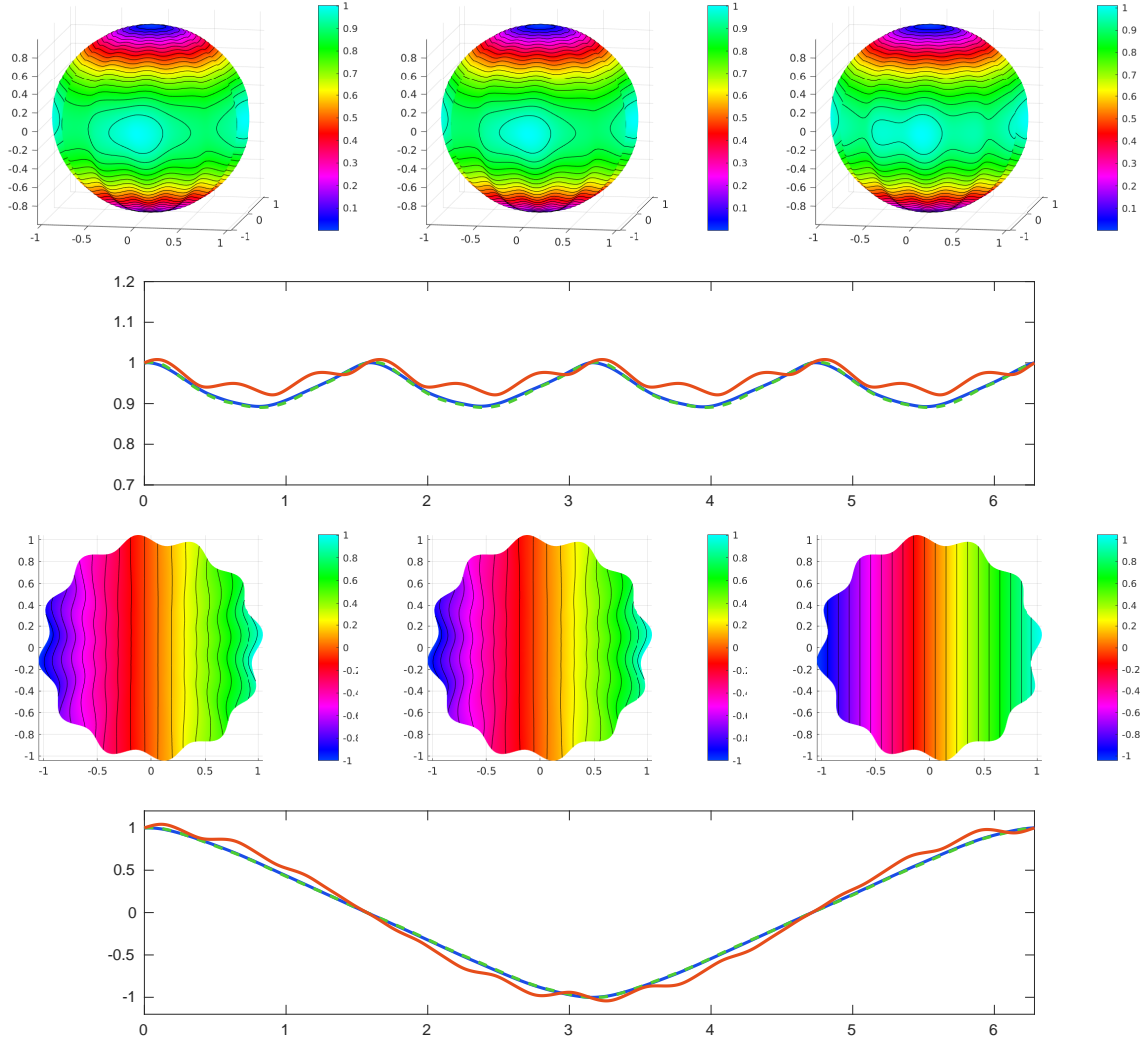


Figure 6.8: First and third row: Results of extrapolation based on Hessian energy (left) and Laplacian energy (mid) as well as restriction of a standard $\mathbb{P}_{3,2}$ -extrapolation (right), all accompanied by isolines. Second and fourth row: evaluations of extrapolation on the equator, for Hessian energy (blue), Laplacian energy (green) and $\mathbb{P}_{3,2}$ -extrapolation (orange). As usual, presented as unrolled on standard interval $[0, 2\pi]$ for arc-length proportional parameterisation.

actually little difference between them. And we see that in particular the equator evaluation of both results is essentially symmetric, which would not be the case if we had serious artifacts by the ESM that was itself unsymmetric — recall that it was only rotation symmetric, but not reflection symmetric as the function values are. This becomes particularly clear if we compare the result to standard extrapolation in the ambient space by polyharmonic spline $\mathbb{P}_{3,2}$ in the respective data sites that actually reduces to a linear polynomial in the second case: If this interpolant is evaluated on the ESM and the equator, we encounter precisely these artifacts. We would further like to emphasise that the “top view” on the second example visualises the fact that the results of our new extrapolation have isolines that are

intrinsically of about the same distance, while for the restricted interpolation that knew nothing about the ESM these have extrinsically the same distance.

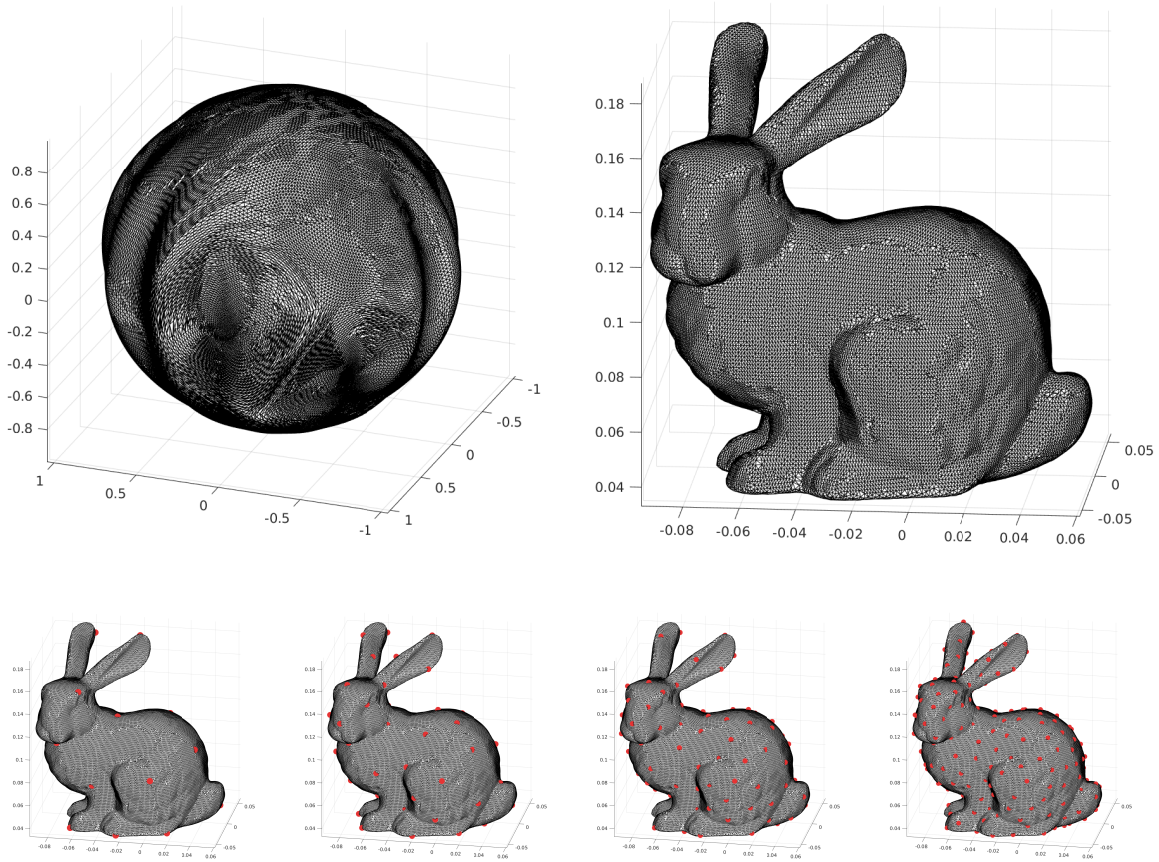


Figure 6.9: Upper row: Parameter space “pumpkin” (left) for the stanford bunny (right). Lower rows: Samplings of the stanford bunny model with different amounts of data, increasing from left to right.

The other example is comparably nonstandard: One can get from [65] a scattered data parameterisation of the *stanford bunny* as a function of the sphere S^2 , due to an algorithm of [85]. This parameterisation was, for example, used in [74] for approximation by the *Ambient B-Spline Method*. By an easy projection operation, we can transfer this parameterisation onto the “pumpkin”: the latter is star-shaped and allows for projection onto S^2 and vice versa. Consequently, we get the bunny as a function of the pumpkin, as depicted in Fig. 6.9. And although this modeling approach is not what we have in mind as the prime objective of our method, we found it reasonable as an easy and impressive visualisation of the effect of our concepts, see Fig. 6.10. We have used samples of 21, 55, 112, and 248 data sites, depicted in Fig. 6.9.

Considering the results depicted in Fig. 6.10, we see that again essentially no relevant difference between Laplacian and Hessian energy is present, and that the

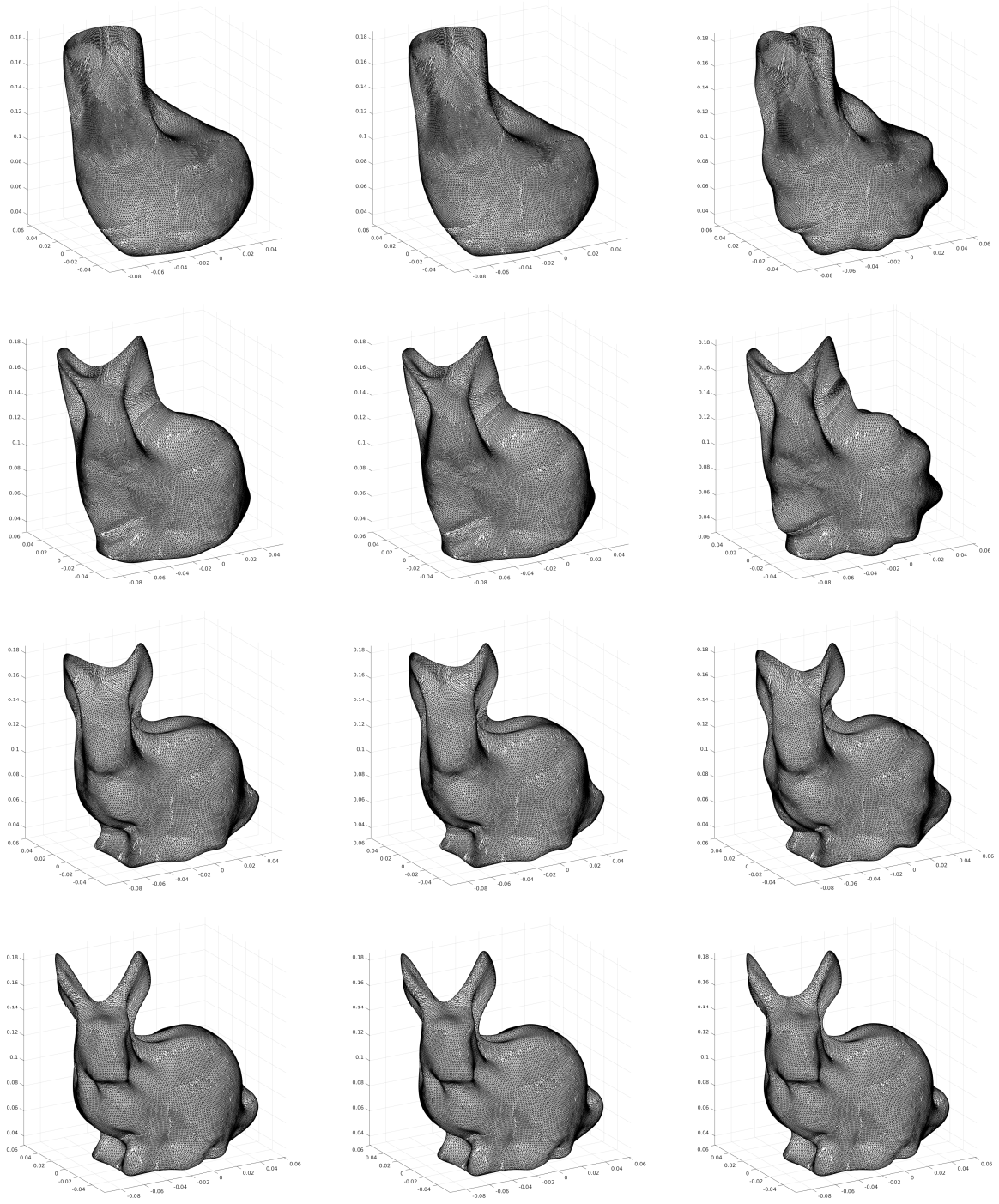


Figure 6.10: *First column: Extrapolation by APA based on Hessian energy to sites of Fig. 6.9. Second column: Extrapolation by APA based on Laplacian energy to sites of Fig. 6.9. Third column: Extrapolation mere restriction of $\mathbb{P}_{3,2}$ interpolation to sites of Fig. 6.9.*

bunnys shape becomes more and more visible the more data sites are used, as one would expect. Furthermore, comparing our method to simple restriction of a $\mathbb{P}_{3,2}$ interpolation, we see that particularly for sparse sites the advantage is significant, while it gets more and more lost if the data becomes denser. This is in fact what we

would expect not only by the convergence results of [49] for RBF interpolation in increasingly dense data sites, but also from a geometric point of view: The denser the data becomes, the more the largest region without any data sites will approach being "flat", whereby the geometry of the ESM becomes increasingly irrelevant.

6.6 Remark: (1) At this point, it should be noted again that this method is not designed for large amounts of data sites. This would require far too many degrees of freedom to meet interpolation constraints and provide at the same time sufficient decrease in normal derivatives. In our tests, we found it particularly difficult to achieve pleasant results once we have, roughly speaking, more than one data site per active cell. In such cases, the interpolation constraints consumed too many of the degrees of freedom to leave enough approximation power for reasonable function values "in between". And further, from a certain point on it may simply be more efficient to use methods like that of [49] than extrapolation on dense data sites, because the system — though sparse — contains the energy matrix and one row and column per interpolation constraint.

(2) Whenever extrapolations of several sets of function values for the same set of data sites has to take place, it will prove beneficial to make use of a suitable Lagrangian basis for these data sites in the extrapolation.

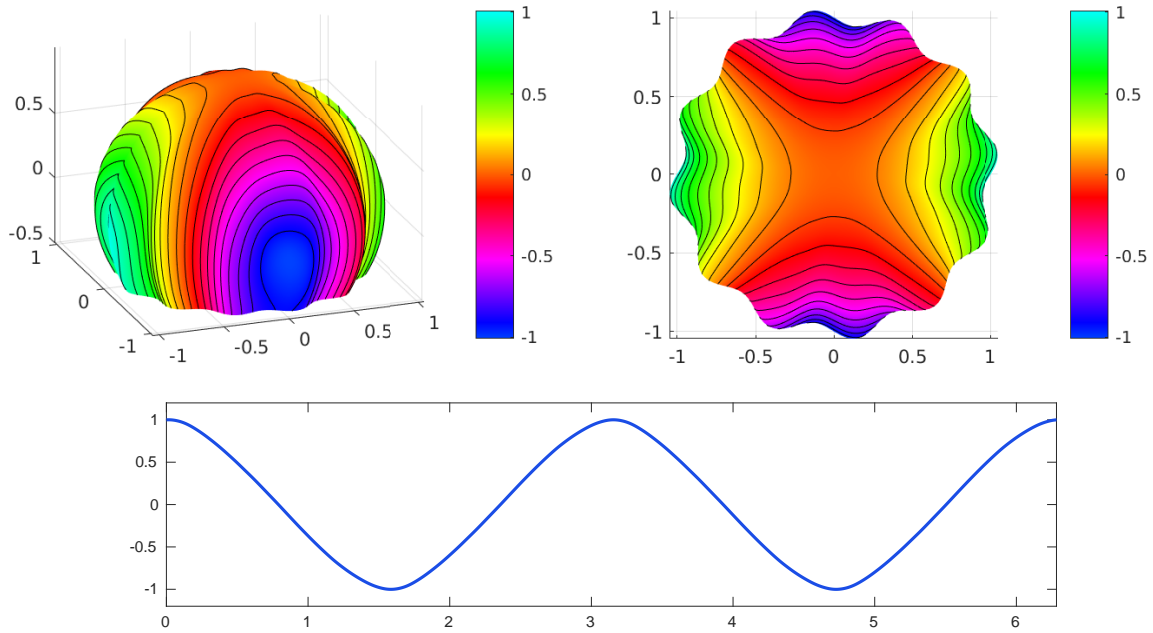


Figure 6.11: Upper row: Evaluation of the cut pumpkin extrapolation, seen from the side and from above. Lower row: Evaluation of the extrapolation on the pumpkin equator. As usual, presented as unrolled on standard interval $[0, 2\pi]$ for arc-length proportional parameterisation.

Ultimately, we also present an example of extrapolation on a surface with boundary: We simply cut off the lowest quarter of the pumpkin. Then we impose the interpolation constraints

$$(1, 0, 0) \mapsto 1, (0, 1, 0) \mapsto -1, (-1, 0, 0) \mapsto 1, (0, -1, 0) \mapsto -1, (0, 0, 1) \mapsto 0.$$

Clearly, this configuration gives us sufficient unisolvency, as the resulting surface is not developable. The resulting evaluation on the whole surface and on the pumpkin equator is again symmetric and free of any serious artifacts induced by the geometry for the Hessian energy. In particular, the evaluation is again essentially reflection symmetric, while the surface is not.

6.2 Smoothing with Scattered Data Sites

In the previous section, we investigated extrapolation from exact data that corresponds to the ideas of periodic and natural cubic splines. In this section, we are going to look at situations where the function values in the data sites are noisy or a smoother solution than implied by the given function values is desired for some other reason — so a setting that corresponds to the objective of smoothing splines. Like in the previous section, we have actually everything prepared for this, and just need to “insert” things appropriately. First of all, the intrinsic energy functional of choice is now

$$\mathcal{E}_\eta^\Xi(f) := \eta \cdot \mathcal{E}_H(f) + (1 - \eta) \cdot \sum_{\xi \in \Xi} (f(\xi) - y(\xi))^2$$

or a suitable adaption of it. In particular, we recall that we can replace the constant η by a smooth, bounded, positive function η on the integral side and by suitable pointwise positive weights $\mathbb{H}_\Xi = \{\eta_\xi\}_{\xi \in \Xi}$ to obtain

$$\mathcal{E}_{\mathbb{H}, \eta}^\Xi(f) := \int_{M_0} \eta \cdot \mathcal{E}_H(f) + \sum_{\xi \in \Xi} \eta_\xi \cdot (f(\xi) - y(\xi))^2.$$

As stated previously and easily verified, this remains continuous and coercive. This specific choice aims at situations where either smoothness requirements or the relevance of approximation in certain data sites varies. In particular, it can be used to overcome irregular samplings to some degree, putting more stress on data sites in sparse regions and less stress on those in dense regions, e.g. clusters. As in the last section, we could replace the Hessian energy by Laplacian energy on any compact ESM.

In any case, we can directly identify these functionals with their corresponding expressions in terms of tangent directional derivatives and deduce the corresponding APA minimisation functionals of the form

$$\begin{aligned} P_{\Xi, M_0}^\eta(S, \sigma_M, \sigma_C) &:= \mathcal{E}_\eta^{\mathbb{T}, \Xi}(S) + h^{-\sigma_M} N_M^\nabla(S, M_0) + h^{-\sigma_C} N_C^\nabla(S, M_0), \\ P_{\Xi, M_0}^{\mathbb{H}, \eta}(S, \sigma_M, \sigma_C) &:= \mathcal{E}_{\mathbb{H}, \eta}^{\mathbb{T}, \Xi}(S) + h^{-\sigma_M} N_M^\nabla(S, M_0) + h^{-\sigma_C} N_C^\nabla(S, M_0), \end{aligned}$$

for the tangent directional counterparts $\mathcal{E}_\eta^{\mathbf{T},\Xi}, \mathcal{E}_{\mathcal{U},\eta}^{\mathbf{T},\Xi}$ of $\mathcal{E}_\eta^\Xi, \mathcal{E}_{\mathcal{U},\eta}^\Xi$ on \mathbf{M}_0 . As in the last section, we can and will replace $C_h(\mathbf{M}_0)$ in practice by suitable supersets: Instead of $C_h(\mathbf{M}_0)$, we use all cells whose center has distance at most h to the considered subdomain $\mathbf{M}_0 \Subset \mathbf{M}$, and all the basis functions active on these.

We first verify the validity of the concept by investigating the behaviour for different parameters on an open and on a closed curve, depicted in Fig. 6.12. The results are also depicted in Fig. 6.12, indicating validity.

6.7 Remark: Because the factor η in $\eta \cdot \mathcal{E}_H(f)$ has an impact on the relation of $\mathcal{E}_H(f)$ to the penalty, it is in practice often convenient to change $\mathcal{E}_\eta^\Xi(f)$ to

$$\mathcal{E}_H(f) + \frac{1-\eta}{\eta} \cdot \sum_{\xi \in \Xi} (f(\xi) - y(\xi))^2$$

in the APA functional, in particular when η is small. This does no harm to solvability and convergence, and it can improve the results substantially for small η if comparably few basis functions are available. Of course, it means in fact just to use some positive weight $\tilde{\eta} = \frac{1-\eta}{\eta}$ on the function value error.

Following these initial considerations, we turn to a short analysis of the convergence behaviour. First of all, we make use of the fact that the optimum is again known for curves, namely it is again a natural (or periodic) cubic spline to the respective arc-length-parameterised (or at least arc-length-proportional) curve, and the knots are precisely the smoothing sites. Just the data values of the spline interpolation are different this time.

As in the last section, we can expect the optimum again to be at least $H^{3.5-\varepsilon}(\mathbf{M})$ by our regularity considerations for univariate splines, and therefore can make the same choices for the penalty exponents σ_M and σ_C as in case of extrapolation. By our theory, we can thus expect the same theoretical upper bound on the convergence order as in case of extrapolation, and in fact it turns out that we again have also a comparably better convergence behaviour in practical terms. The tests were performed for the curves and exemplary functions depicted in Fig. 6.13, while the resulting convergence plots are provided in Fig. 6.14.

As in the last section, we use primarily the energy norm to measure the convergence behaviour. But this time we have to consider function values in the sites as well, because we have no strict interpolation constraints and therefore the "function value part" of the energy norm is not constant over all functions. So we use a suitably discretised version of

$$\frac{1}{\int_{\mathbf{M}} 1} \sqrt{\mathcal{E}_H(s_h - s^*)} + \sqrt{\sum_{\xi \in \Xi} (s_h(\xi) - s^*(\xi))^2}$$

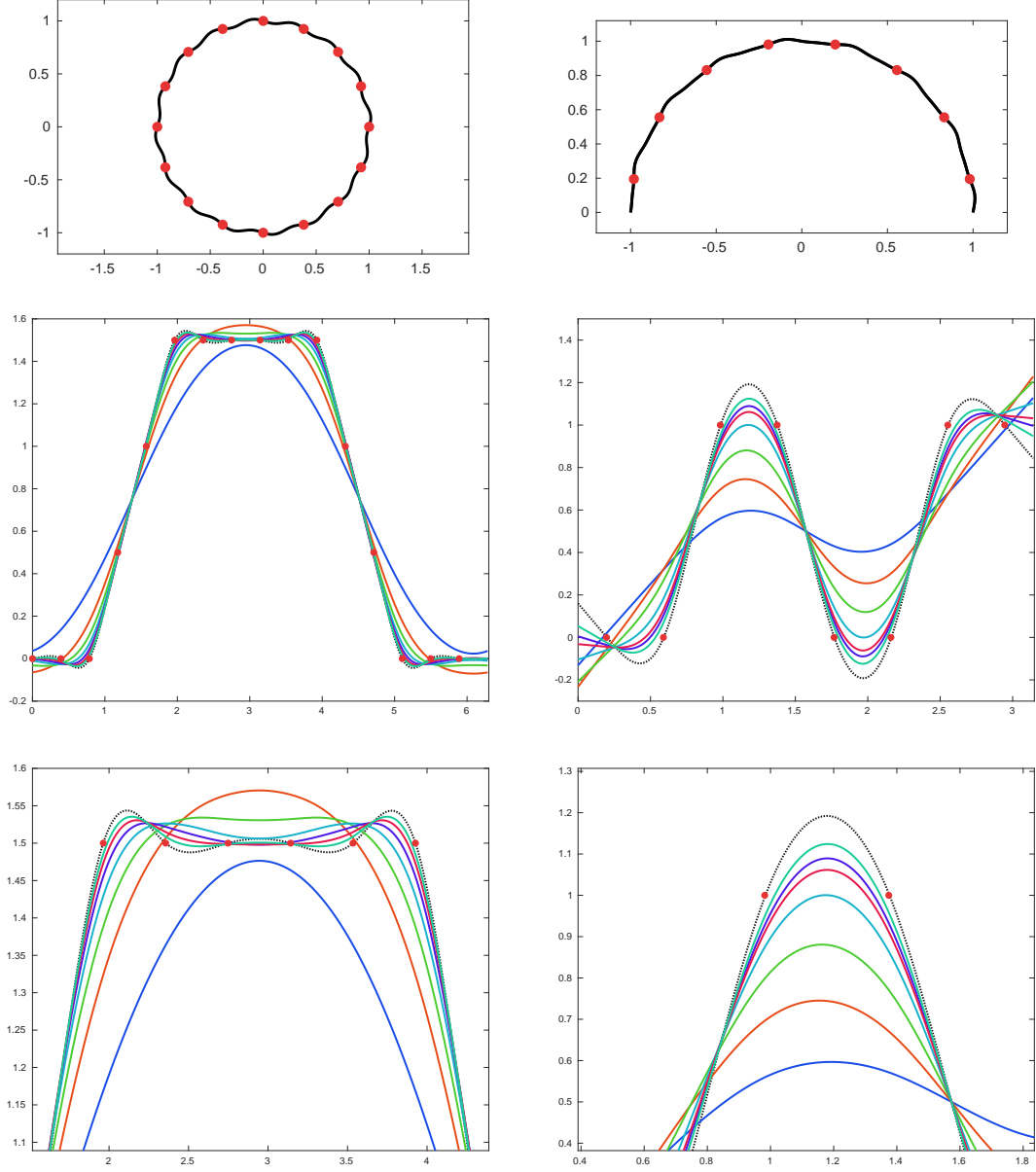


Figure 6.12: First row: Closed (left) and open (right) curve with sample sites. Second row: The smoothing results for different weights along with the initial choice of the data sites to the respective curves, for penalty exponent $\sigma = 2$. As usual, depicted as arc-length proportional parameterisations over standard intervals $[0, 2\pi]$ and $[0, \pi]$. Closed curve sample values: $0, 0, 0, \frac{1}{2}, 1, \frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \frac{3}{2}, \frac{3}{2}, 1, \frac{1}{2}, 0, 0, 0$. Open curve sample values: $0, 0, 1, 1, 0, 0, 1, 1$. In both plots, the sites are depicted in red, the result of extrapolation is depicted in dotted black, and the smoothing results are depicted in blue, orange, green, cyan, violet, purple and teal for increasing emphasis on the function values. Third row: Close-Ups of the different results.

for the APA result s_h and the optimum s^* . Further, we use a correspondingly normalised energy also in the implementation for the sake of comparability, so we multiply all integrals by $1/\text{vol}(\mathcal{M})$. And as before and depicted in Fig. 6.14, the actual convergence behaviour seems to be at about $h^{3/2}$ to h^2 with a saturation that

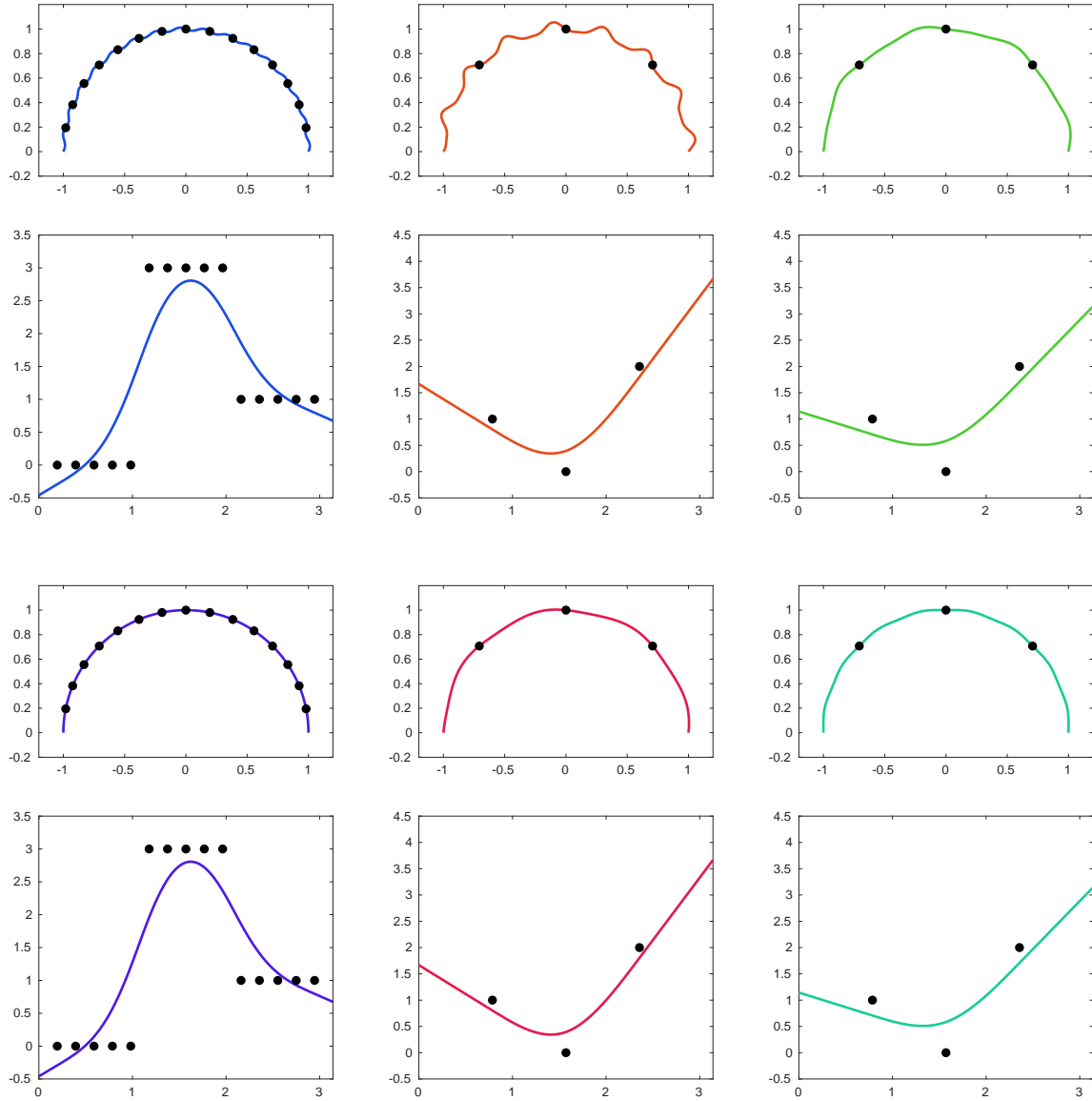


Figure 6.13: Exemplary curves with data sites and corresponding smoothing spline functions that appear as optimal solutions for APA minimisation.

occurs at least below 10^{-3} , and also the L_2 seems to converge at least quadratically until saturation at about 10^{-4} to 10^{-6} .

However, in the current situation the choice $\sigma_M = 2$ apparently outperforms the choice $\sigma_M = 3$: An explanation for this seems to be that as the function values are part of the functional this time, the numerical dominance of the penalised part now affects the way the function values in the sites are considered by the functional more directly: The function values become increasingly irrelevant from a numerical point of view, and therefore the approximations saturate earlier and less satisfactory in the rms, while the energy error is surprisingly little affected

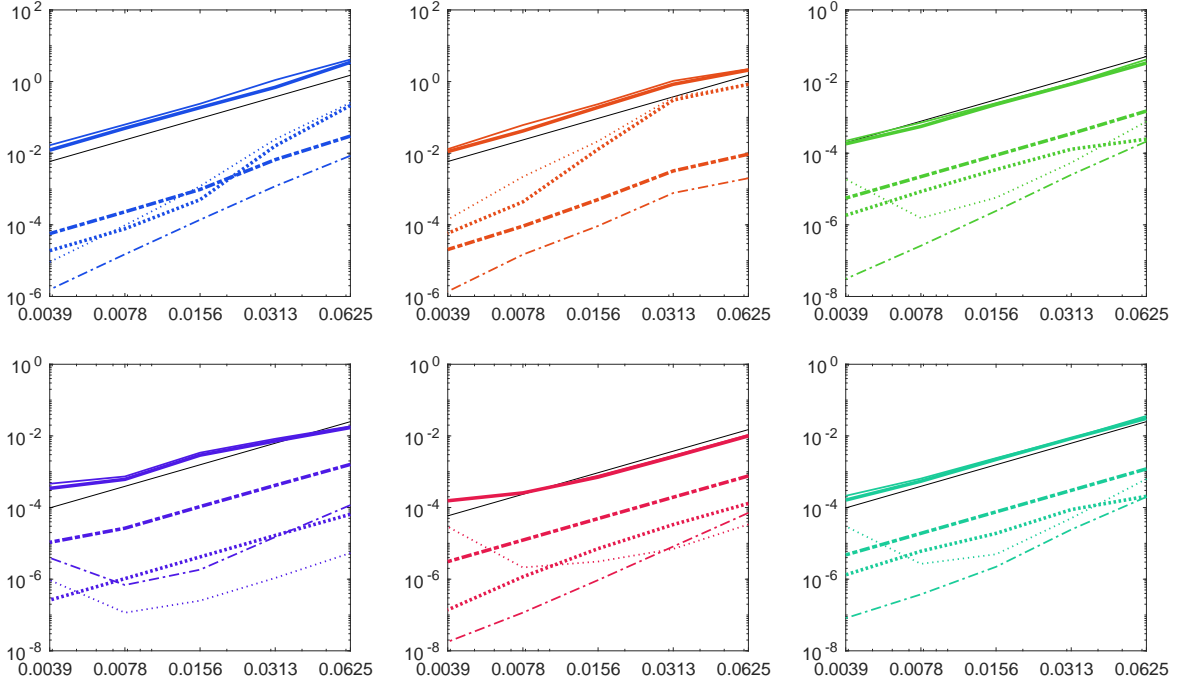


Figure 6.14: Convergence order plots for the data of the last figure: Solid is the energy, dot-dashed the normal derivative, dotted the L_2 error for about $300[1/h]$ points. The thicker lines refer to $\sigma_M = 2$ and the thinner lines to $\sigma_M = 3$, while we chose in both cases $\sigma_C = 2$. Reference h^2 is depicted in solid thin black.

by this; that effect is actually also the reason why we depicted $\sigma_M = 2$ bolder this time, with thinner $\sigma_M = 3$ for the sake of comparison.

Now we will again turn to surfaces, where we choose once again $\sigma = \sigma_M = \sigma_C = 2$ as in the extrapolation case for surfaces. In our first example, we make use of the stanford bunny once more and sample it in 1'414 sites depicted in Fig. 6.15, and we provide smoothened versions of the approximation for different smoothing factors. In this example we use $h = 0.125$, whereby about 6'000 basis functions are employed in the minimisation functional.

We see in Fig. 6.16 that while we start with something that is not much more than a "blob", the actual shape of the bunny becomes more and more visible with increasing emphasis on the data sites, until we have reached a version of the bunny that is almost a product of interpolation.

Moreover, we also exemplify the smoothing power of this approach on an open surface with boundary, namely the upper half of the unit norm ball in the 6-norm, so the zero-surface of

$$x^6 + y^6 + z^6 - 1, \quad x, y, z \in \mathbb{R}, z \geq 0.$$

On this surface, we sample 857 (roughly) uniformly distributed data sites Ξ and as-

sign uniform noise from $[-\frac{1}{2}, \frac{1}{2}]$ to the sites. That noise is then added to evaluations of the function

$$(x, y, z) \mapsto x^2 + y^2$$

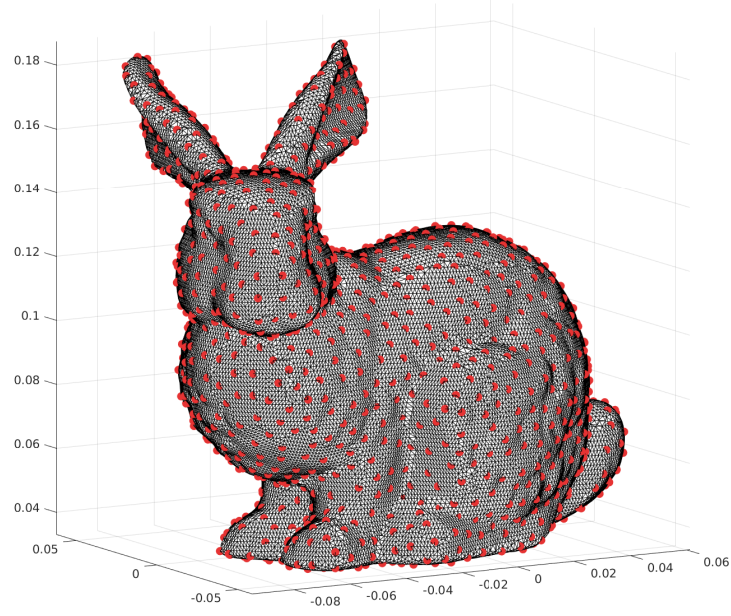


Figure 6.15: *Bunny with sample sites.*

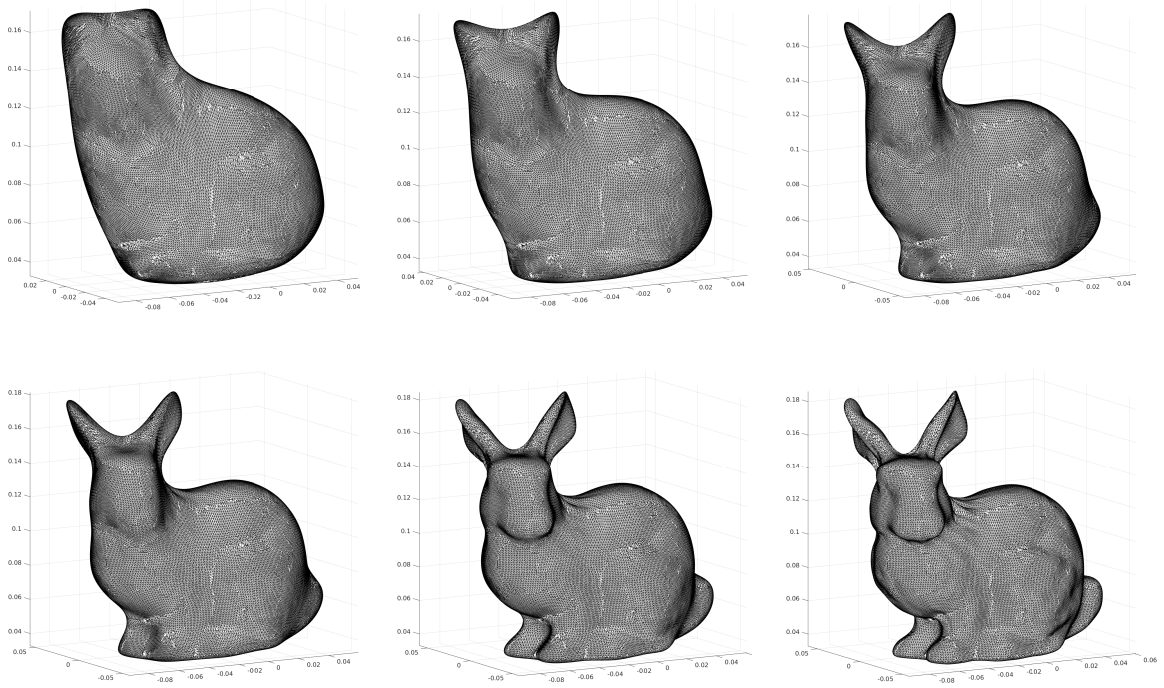


Figure 6.16: *"Smoothened" stanford bunny, emphasis on the data site function value increasing.*

in the data sites to obtain noisy function values. These noisy function values will then provide Y_{Ξ} in the APA smoothing functional.

We obtain for different weights (the emphasis on smoothness increases by a factor of about 3 in each step) different levels of smoothing, depicted in Fig. 6.17. Note that in particular for higher emphasis on smoothness the results are quite satisfactory, particularly when considering the significant original noise.

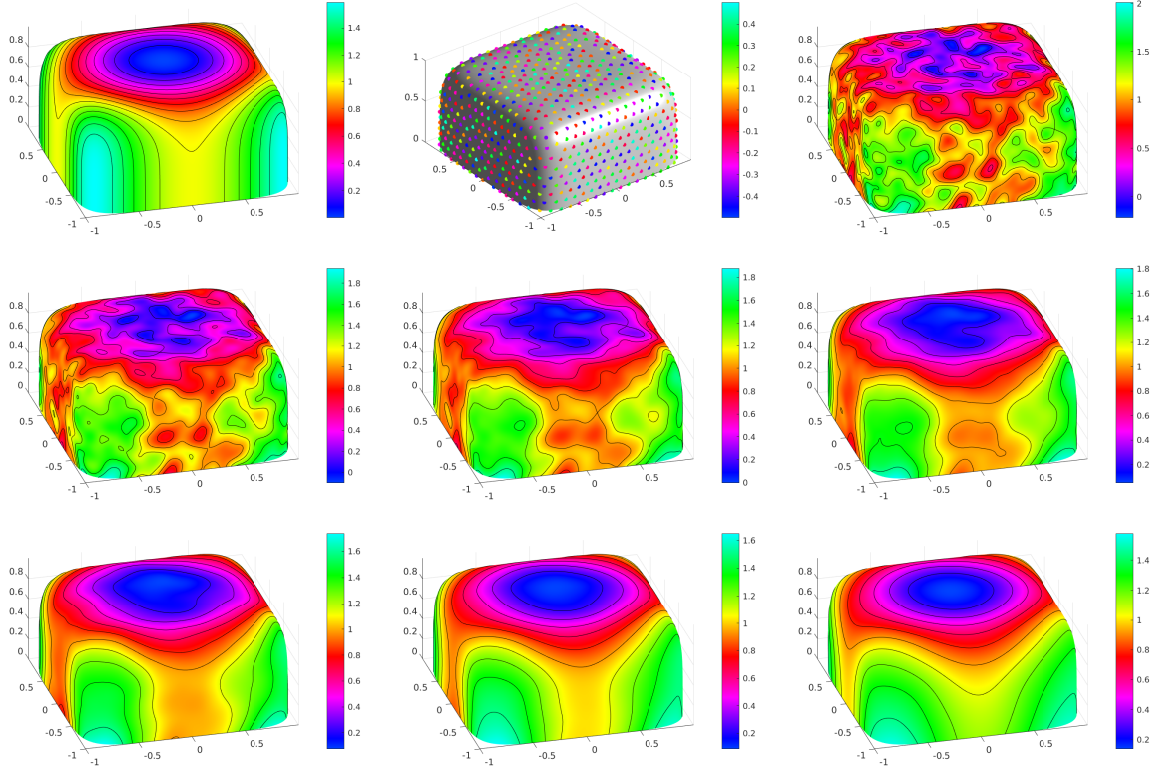


Figure 6.17: First picture: Surface with original function $(x, y, z) \mapsto x^2 + y^2$. Second picture: Surface with 857 data sites and measurement error there. Other pictures: Results for smoothing with different smoothing weights, starting with a high emphasis on function values.

Finally, we suppose to be in a more difficult situation: The data sites are no longer uniformly distributed, but cluster around $(0, 0, 1)$, and additionally the measurement errors are higher in the clustered area. These are typical situations for point-wise weighting, resembling the data density and / or the known information on local error distributions or the like.

In our example, we can handle both by the same, as we suppose to know that the measurement error increases with the density, and we handle them by simply weighting each site $\xi \in \Xi$ with the inverse count of data sites within the Euclidean ball around ξ that has radius

$$r_0 = \frac{1}{2} \max_{\xi \in \Xi} \min_{\substack{\zeta \in \Xi \\ \zeta \neq \xi}} \|\xi - \zeta\|_2.$$

We use this just to exemplify the concept, the actual choice of the pointwise weighting is then of course depending on the specific circumstances of the actual problem. The results, for 890 clustering sites, are depicted in Fig. 6.18. There, it becomes particularly obvious that the local weighting can provide significant advantages over uniform weighting (which is depicted in the last row of the figure for the sake of comparison).

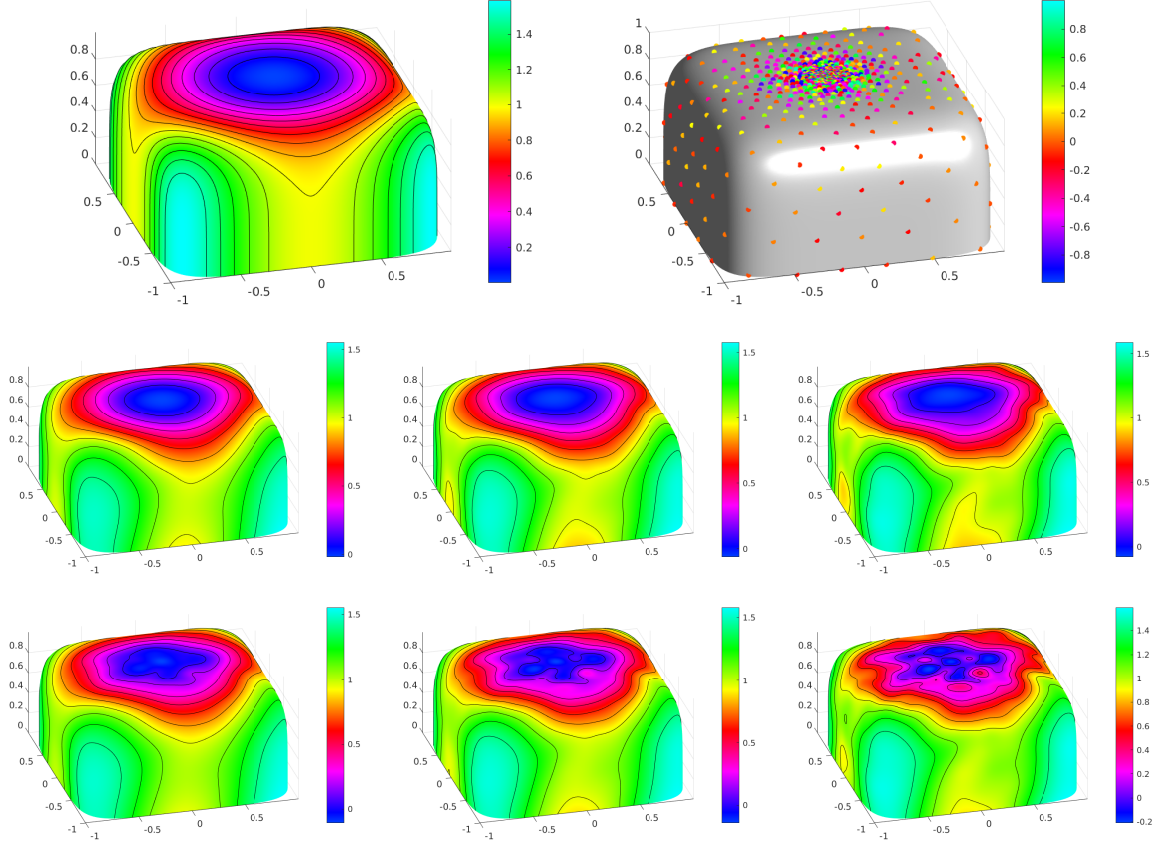


Figure 6.18: First row: Initial function (left) and surface with 890 clustering data sites and error in those sites (right). Second row: Results for certain global smoothing weight with local weighting. Third row: Results for certain global smoothing weight with uniform weighting.

6.3 Irregular Samplings

In the first section, we have proposed a novel approach for extrapolation of function values in sparsely sampled data sites. While this was already an intricate task in its own right, things become even more challenging when the sampling is irregular, and we have both regions with sparse (or almost no) and regions with comparably dense sampling.

The idea we propose is to use a bilevel approach, where in the first level the extrapolation method of the first section in this chapter is applied to some sparse subset

of the given set Ξ . In a second level, this approximation is then refined by suitable local approximations in the densely sampled regions. But to accomplish the latter, we need an approximation method for the second level!

It could be based on ideas of [49], where restriction of radial basis function interpolations to an ESM is proposed. This concept provides promising convergence behaviour and a certain degree of independence from the respective submanifold, in particular it is applicable to subdomains without any further requirements. But for a reasonable overall solution after both levels we would have to require the second level to provide a TP-spline function as well — whereby we would also gain the favorably cheap evaluation of splines for the overall solution. To achieve this, one can choose to combine the approach of [49] and TP-splines by a so-called *two-stage method*.

6.3.1 A Two-Stage Approximation Approach

The idea of such an approach is to construct an approximation by two subsequent approximation steps: The first stage produces some (possibly local collection of) approximant(s). This is then itself reapproximated in the second stage to obtain the final solution. It therefore stands in the tradition of various *two-stage* or *multi-stage* schemes, dating back to the seventies at least (cf. e.g. [90]) and presented in various subsequent variants (cf. [23] - [24], [42]). There, the first stage is usually of local nature, in order to reduce the computational complexity, while we restrict ourselves here to the case of a global first stage for the sake of simplicity, in particular in the error analysis; the following considerations should only serve as a “proof of concept” that also in the manifold situation such an approach is viable and reasonable.

We propose to use interpolation by radial basis functions as presented in [49] in the first stage, and quasi-projection by TP-splines in the second, and we shall give a short convergence analysis of the matter here. To accomplish that, we will first have to give a very brief revision of some radial basis function theory.

We have already seen an important example, namely the polyharmonic splines, and these have already illustrated the basic idea: Take a suitable univariate function $\phi : [0, \infty[\rightarrow \mathbb{R}$ and make a multivariate function $\Phi : \mathbb{R}^d \rightarrow \mathbb{R}$ out of it by applying it to suitable norm⁽²⁾. Thereby, one obtains $\Phi(x) = \phi(\|x\|)$, and these functions ϕ and Φ have to meet certain additional requirements (cf. [105, Ch. 8,9]), most of which lie beyond the scope of this thesis. We just remark here that under suitable conditions

⁽²⁾usually either the Euclidean norm $\|\cdot\|_2$ or a suitably transformed Euclidean norm $\|\cdot\|_T := \|T(\cdot)\|_2$ for a linear isomorphism $T : \mathbb{R}^d \rightarrow \mathbb{R}^d$, cf. e.g. [12, 17, 19, 20, 40, 105]

on the coefficients, on the distribution of data Ξ and possible enhancement by a low-degree polynomial (cf. [105, Ch. 6-9]), there is a unique function of the form

$$\phi_{\Xi, Y} := \sum_{\xi \in \Xi} a_{\xi} \Phi(\cdot - \xi) + \sum_{i \in I} P_i(\cdot)$$

that interpolates function values Y_{Ξ} in points of Ξ , wherein the $\{P_i\}_{i \in I}$ form a basis of the respective low-degree polynomial space. Thereby, the algorithmic description of our method can directly be given as follows:

6.8 Algorithm — Two-Stage Approximation Method —

1. Determine a spline grid of width h and order m , and choose all cells active on a given ESM or a small tubular neighbourhood of it.
2. For each B-spline b_{ℓ} active on an active cell, determine a suitable set Ξ^{ℓ} of data sites from initial Ξ .
3. Calculate the RBF interpolant $\phi_{\Xi^{\ell}, Y^{\ell}}$ for that set Ξ^{ℓ} and corresponding function values Y^{ℓ} .
4. Perform quasi-projection on objective $\phi_{\Xi^{\ell}, Y^{\ell}}$ to determine the coefficient of b_{ℓ} .
5. Combine the resulting coefficients to an overall solution.

This algorithm allows, up to this point, also local approximations by RBF: One can choose the data sites employed to determine the coefficient of a particular B-spline just from a region around the cell or cell center, and the diameter of this region can be chosen proportional to the cell diameter. For the upcoming convergence analysis, we will however restrict ourselves as announced to one global RBF approximation in the first step for the sake of simplicity. In our tests, we found that suitable localisations would still yield satisfactory results, but a detailed analysis of this situation would lead to far here.

6.9 Remark: (1) The advantage of the global approach is that the RBF approximation needs only to be calculated once, but this system may be (very) large, while the local approach requires multiple solutions of, yet considerably smaller, systems. The global approach is therefore problematic if the number of data sites is very large (say, more than 10'000 points), while it is favorable for medium sized problems (say, less than 10'000 points), as in this case the solution of one system of at most 10'000 coefficients is presumably more efficient than solving local systems of still several hundreds of coefficients for several thousand B-splines if parallelisation is not employed excessively.

(2) The advantage of this two-stage approach over any direct spline approximation method is that the spline step does not have to face the ESM. In particular, it does not face the boundary of an open ESM, whereby no problems with boundary cells

can arise. Instead, it does only require the RBF approximation, which is theoretically available on all of \mathbb{R}^d , although in the end only evaluations near the ESM are required. Moreover, in the end only spline basis functions and coefficients for cells active on the ESM have to be stored, as in the ambient B-spline method.

There are numerous choices for ϕ , but we shall restrict ourselves just to the well-known compactly supported *Wendland functions* $\Phi_{d_0,m}$ for the choice $\phi_{d_0,m}$ of the univariate function, admissible for suitable dimensions $d \leq d_0$ and depending on some additional parameter m as given in [105, Ch. 9] with prominent examples

$$\begin{aligned} \phi_{1,1}(t) &= (1-t)_+^4(4t+1) & \in C^2 & \quad (d \leq 1) \\ \phi_{3,2}(t) &= (1-t)_+^6(35t^2+18t+3) & \in C^4 & \quad (d \leq 3) \\ \phi_{3,3}(t) &= (1-t)_+^8(32t^3+25t^2+8t+1) & \in C^6 & \quad (d \leq 3) \\ \phi_{5,1}(t) &= (1-t)_+^5(5t+1) & \in C^2 & \quad (d \leq 5) \\ \phi_{5,2}(t) &= (1-t)_+^7(16t^2+7t+1) & \in C^4 & \quad (d \leq 5) \end{aligned}$$

For these, an additional scaling factor can be used to affect the size of the support: division of the argument by $\delta > 0$ rescales the support to δ . Any of these choices yields different properties w.r.t. approximation power, stability of the interpolation system and others (cf. [105, Ch. 11, 12]). What makes this choice so favorable in our theory is that these functions satisfy a certain "optimality" under all interpolants in suitable Sobolev spaces (cf. [105, Sect. 10.5, Thm. 13.2])⁽³⁾:

6.10 Proposition *For the featured RBF $\Phi_{d_0,m}$ and any $\Xi \subseteq \Omega$ with $\Omega \in \mathbb{Lip}_d^*$, there is a constant $c > 0$ depending on the choice of d_0 and m such that the interpolant $\phi_{\Xi,Y}$ satisfies*

$$\|\phi_{\Xi,Y}\|_{H^{(d+1)/2+m}(\Omega)} \leq c \|f\|_{H^{(d+1)/2+m}(\Omega)}$$

for any $f \in H^{(d+1)/2+m}(\Omega)$ such that $f(\xi) = \gamma_\xi$ for all $\xi \in \Xi$, as long as $1 \leq d \leq d_0$.

On any ESM M , we have the following nice convergence result due to [49]. It was actually proven for compact ESMs alone, but the proof does not feature any relevant properties of compactness and directly generalises to our concepts for Sobolev spaces on open ESMs as subdomains of compact ESMs:

6.11 Proposition *Let $M \in \mathbb{M}_{bd}^k(\mathbb{R}^d)$, $\Phi_{d_0,m}$ as above with $d \leq d_0$ and $\Phi_{M,m}$ its restriction to M . Let further $\varrho = \frac{d+1}{2} + m - \frac{d-k}{2} = m + \frac{k+1}{2}$ and $\sigma \in [0, \infty[$ such that $0 \leq \sigma \leq \varrho$. Then for all $\Xi \subseteq M$ finite s.t. $h_{\Xi,M}$ is sufficiently small and any $f \in H^\varrho(M)$*

$$\|f - T_M \phi_{f,\Xi}\|_{H^\sigma(M)} \leq c \cdot h_{\Xi,M}^{\varrho-\sigma} \|f\|_{H^\varrho(M)},$$

⁽³⁾In fact, other choices have similar optimality properties in their respective so-called *native space*, just we do not address the matter of native spaces here any further for the sake of brevity.

where $\phi_{\Xi, f}$ is the interpolant to f obtained as $\phi_{\Xi, Y}$ for $Y_{\Xi} = \{y_{\xi} := f(\xi), \xi \in \Xi\}$ and $h_{\Xi, M}$ is defined for the distance $d_M(\cdot, \cdot)$.

Proof: One only needs to verify that no features of compactness of M were ever used in the proof of [49, Lemma 10, Thm. 11] once a suitable finite inverse atlas like ours is provided, and to replace [49, Prop. 9] by [106, Thm. 4.6], both of which can be accomplished easily. \square

We obtain thereby almost immediately the convergence order for the corresponding two-stage approximation on a single, fixed region covering the whole ESM:

6.12 Theorem *Let $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ be sampled in some set $\Xi \subseteq M$. Let $f \in H^{\varrho}(M)$ with $\varrho = \mu + (k + 1)/2$ for the choice $\Phi_{d_0, \mu}$ with $d \leq d_0$, and let $\phi_{\Xi, f}$ be the corresponding interpolation to f in Ξ . Let $S_{h, \Xi}$ be the TP-spline quasi-projection of order $m \geq \mu + (d + 1)/2 + 1$ to $\phi_{\Xi, f}$ in \mathbb{R}^d , and let $s_{h, \Xi}$ be its restriction to M . Let h and $h_{\Xi, M}$ be sufficiently small. Then for any $0 \leq \sigma \leq \varrho$ and any $\varepsilon \geq 0$ such that $\max(\varepsilon, \sigma) > 0$*

$$\|f - s_{h, \Xi}\|_{H^{\sigma}(M)} \leq c \cdot (h^{\varrho - \sigma - \varepsilon} + h_{\Xi, M}^{\varrho - \sigma}) \|f\|_{H^{\varrho}(M)}.$$

All statements remain valid in limiting cases $\mu + (d + 1)/2 \leq m < \mu + (d + 1)/2 + 1$ under the following conditions:

$$1. \ d \text{ odd, } m = \mu + (d + 1)/2 \in \mathbb{N} \text{ and } \sigma + (d - k)/2 \leq m - 1. \quad (6.12.I)$$

$$2. \ d \text{ even, } m = \mu + (d + 2)/2 \in \mathbb{N}, \sigma + (d - k)/2 < m \text{ and } \varepsilon > 0. \quad (6.12.II)$$

Proof: By the triangle inequality we have

$$\|f - s_{h, \Xi}\|_{H^{\sigma}(M)} \leq \|f - T_M \phi_{\Xi, f}\|_{H^{\sigma}(M)} + \|T_M \phi_{\Xi, f} - s_{h, \Xi}\|_{H^{\sigma}(M)}.$$

Due to convergence results for restricted RBF interpolation the first term in that relation satisfies

$$\|f - T_M \phi_{\Xi, f}\|_{H^{\sigma}(M)} \leq c h_{\Xi, M}^{\varrho - \sigma} \|f\|_{H^{\varrho}(M)},$$

so we have to make further efforts for the second term only. There, we first restrict ourselves to the case $m \geq \mu + (d + 1)/2 + 1$ and set $r := \varrho + (d - k)/2 = \mu + (d + 1)/2 \leq m - 1$, $\varsigma = \sigma + \frac{d-k}{2}$. Then we find by the trace theorem, the convergence result for quasi-projections of Theorem 3.8 and its particular application to splines in Corollary 3.15 due to $r - \varsigma = \varrho - \sigma$ that whenever $\sigma > 0$ it holds

$$\|T_M \phi_{\Xi, f} - s_{h, \Xi}\|_{H^{\sigma}(M)} \leq \|\phi_{\Xi, f} - S_{h, \Xi}\|_{H^{\varsigma}(\mathbb{R}^d)} \leq c h^{\varrho - \sigma} \|\phi_{\Xi, f}\|_{H^r(\mathbb{R}^d)}. \quad (6.12.1)$$

In case $\sigma = 0$ one obtains for sufficiently small $\varepsilon > 0$ similarly that

$$\|T_M \phi_{\Xi, f} - s_{h, \Xi}\|_{L_2(M)} \leq \|T_M \phi_{\Xi, f} - s_{h, \Xi}\|_{H^{\varepsilon}(M)}$$

$$\leq \|\phi_{\Xi, f} - S_{h, \Xi}\|_{H^{\varsigma+\varepsilon}(\mathbb{R}^d)} \leq c h^{\varrho-\sigma-\varepsilon} \|\phi_{\Xi, f}\|_{H^r(\mathbb{R}^d)}. \quad (6.12.2)$$

In any case, by the (fractional) trace theorem and the universal bounded extension operator $E_M^{\mathbb{R}^d}$ we have

$$\|f\|_{H^\varrho(M)} \leq c_1 \|E_M^{\mathbb{R}^d} f\|_{H^r(\mathbb{R}^d)} \leq c_2 \|f\|_{H^\varrho(M)}.$$

This finally gives the desired result thanks to optimality of RBF interpolation due to Prop. 6.10 via the relation

$$\|\phi_{\Xi, f}\|_{H^r(\mathbb{R}^d)} \leq c \|E_M^{\mathbb{R}^d} f\|_{H^r(\mathbb{R}^d)} \leq c \|f\|_{H^\varrho(M)}.$$

To obtain the corresponding results in the limiting cases (6.12.I) and (6.12.II), we need to modify the relations (6.12.1) and (6.12.2) as follows:

1. If $m = \mu + (d + 1)/2 \in \mathbb{N}$ and $\sigma + (d - k)/2 \leq m - 1$, no adaptations need to be made, but the second statement of Theorem 3.8 for TP-splines needs to be employed.
2. If $m = \mu + (d + 2)/2 \in \mathbb{N}$ and $\sigma + (d - k)/2 < m$, we have $r = \mu + (d + 1)/2$, so an $\varepsilon > 0$ more than the admissible choice due to the regularity of splines. So we deduce for any $\varepsilon > 0$ that by the trace theorem, Theorem 3.8 for TP-splines (so Cor. 3.15) and fractional Sobolev embeddings

$$\|T_M \phi_{\Xi, f} - s_{h, \Xi}\|_{H^\sigma(M)} \leq c h^{\varrho-\sigma-\varepsilon} \|\phi_{\Xi, f}\|_{H^{r-\varepsilon}(\mathbb{R}^d)} \leq c h^{\varrho-\sigma-\varepsilon} \|\phi_{\Xi, f}\|_{H^r(\mathbb{R}^d)},$$

where one needs to replace ε by $\varepsilon/2$ and σ by $\varepsilon/2$ in the further limiting case $\sigma = 0$.

With these adaptations, we can proceed as before to obtain the respective convergence orders for limiting cases. \square

We give now just one example for this, similar to the one chosen in [49]: We consider a "stretched" torus as depicted in Fig. 6.19, and evaluate the function

$$f_0(x, y, z) := \exp(xz) \cdot x \cdot \sin(5xy) \cdot \cos(6yz)$$

at about 100 roughly uniformly distributed sites. Then we compute the Matern-kernel interpolant to these sites and values, as recommended and similarly performed in [49] to obtain a function $f \in H^{4-\varepsilon}(\mathbb{R}^3)$ for any $\varepsilon > 0$. This f is now our *target function* for the approximation. By our choice of regularity of the target function, a suitable choice for the RBF is $\Phi_{3,2}$, which gives again $H^4(\mathbb{R}^3)$ to measure error. So we obtain $\varrho = 3.5$ and we consequently choose spline order 4.

The expected rate of convergence in $L_2(\mathcal{M})$ is then effectively $h^{3.5} + h_{\Xi, \mathcal{M}}^{3.5}$, simply because for any $\varepsilon > 0$

$$\|f - s_{h, \Xi}\|_{L_2(\mathcal{M})} \leq \|f - s_{h, \Xi}\|_{H^\varepsilon(\mathcal{M})} \leq c \cdot (h^{\varrho-\varepsilon} + h_{\Xi, \mathcal{M}}^{\varrho-\varepsilon}) \|f\|_{H^\varepsilon(\mathcal{M})}.$$

We use consecutively 462, 943, 1'836, 3'639 and 6'960 approximately uniformly distributed sites⁽⁴⁾. These are obtained by thinning a dense point cloud of 262'000 points until a certain threshold on the minimal mutual distance of 0.2, 0.14, 0.1, 0.07, 0.05 for any two points was reached. Then we choose corresponding spline cells of length $h = \frac{1}{5}, \frac{1}{7}, \frac{1}{10}, \frac{1}{14}, \frac{1}{20}$, and we find the expected rate of convergence verified.

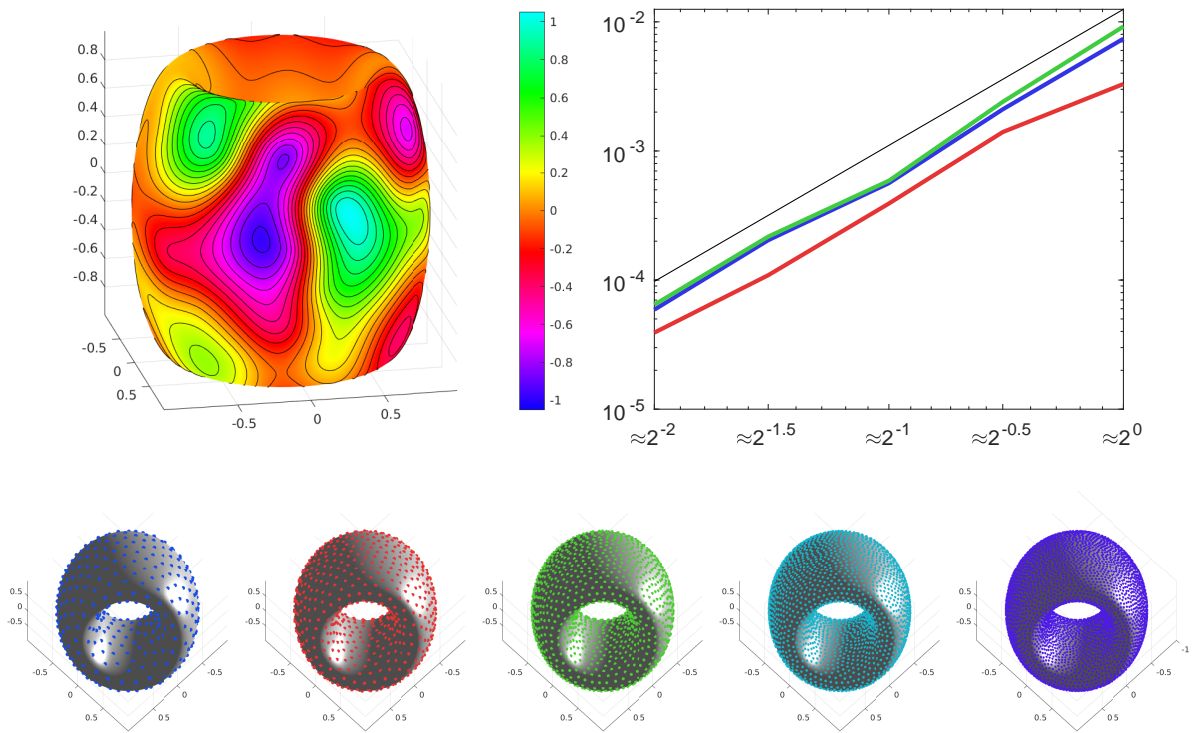


Figure 6.19: First picture: Target function of approximation in the "stretched torus". Second picture: Convergence orders as obtained by root mean square in about 262'000 points. Black: reference $h^{3.5}$. Blue: Two-stage convergence for support radius 3.5. Red: RBF convergence for support radius 3.5. Green: Two-stage convergence for support radius 1.0. Note that the abscissa of the convergence plot is labelled by approximate relations of both fill distance and grid width when compared to initial. Second row: Employed data sites on the surface.

6.13 Remark: (1) It should be noted here that the convergence behaviour depends on which of the two approximation methods is dominant. As there is also a "doubling effect" for the convergence order of radial basis functions if the target function is considerably smoother (cf. [49]), this can lead to improved convergence

⁽⁴⁾In case of a surface, quadrupling the number of (uniformly distributed) sites reduces the fill distance by $1/2$, this means that the fill distance reduces roughly by $1/\sqrt{2}$ in each step.

order until the splines become dominant. Therefore, it can make sense to choose the splines comparably fine, even for comparably sparse sampling of the data sites. (2) We stick to the second approach of Remark 3.14 for the spline quasi-projection, as it provided superior results. There, it also turned out again that we loose nothing on the expected rate of convergence if we consider only cells active on a tubular h -neighbourhood of the ESM instead of all cells in the respective basis function support.

6.14 Remark: Regarding further varieties and modifications of the concept, we can make the following further statements:

- We checked several support radii for the RBF, namely $\delta_{\text{supp}} = 3.5, 2.5, 1.5, 1.0, 0.5$. There appeared no relevant deviation in the error and convergence. We omitted them in the plot because the results were fairly indistinguishable except for 0.5, which produced slightly weaker errors in particular for the sparser sets of data sites, but still the same order.
- The convergence orders were also comparable if we multiplied the length of the spline cells by $\frac{1}{2}$ when compared to the lengths featured above. In that case, we would effectively reproduce the errors of the direct RBF approximation almost exactly.
- We also implemented and tested a corresponding localised version. There, we chose the data sites for each cell by considering only those in a specific ball around the cell center with radius proportional to h . With sufficiently many data sites, the results are still more than pleasant, but we found some mild loss compared to the optimal convergence rate. The behaviour was about that of the global version, just presumably slightly weaker in the end, and yielded for $\approx 28'000$ data sites and $h = 0.025$ a root means square error of $\approx 1.5365 \cdot 10^{-5}$.

6.3.2 A Bilevel Algorithm

With the previous statements in mind, we propose now an approach to handle irregularly sampled data sites. The basic idea is simple and was to some degree inspired by numerous hierarchical and multi-level approaches, e.g. [41, 67, 74]: First, we need a rough solution, obtained by extrapolation via APA minimisation for a thinned subset of the sites, then we calculate the RBF-approximations in the densely sampled areas and apply the quasi-projection method to these. But we use only those spline coefficients whose support contains at least one of the sites in the densely sampled area, while we set the others to zero. Thereby, we exploit

the partition of unity property of the splines to accomplish a smooth blend of the coarse and the fine approximations. We formulate this in a further algorithm now:

6.15 Algorithm — Bilevel Scattered Data Approximation —

1. Determine a subset $\Xi_0 \subseteq \Xi$ that is sufficiently sparse to apply the extrapolation method and roughly uniformly distributed.
2. Apply the extrapolation method from the first section to determine an extrapolation S_0 .
3. Determine the error $\mathcal{E}_0(\Xi) = \{\varepsilon_\xi = \gamma_\xi - S_0(\xi)\}_{\xi \in \Xi}$.
4. Apply the two-stage approximation method, w.r.t. function values ε_ξ in those areas of \mathbb{M} where the data is sufficiently dense to obtain an approximation S_ε .
5. Choose all coefficients from the two-stage solution that belong to basis functions whose support contains a site of a dense region, and create S_ε^* by these coefficients for the respective functions, and zero coefficients for all other functions.
6. Combine the two approximations to overall approximation $S_{\Xi,Y} = S_0 + S_\varepsilon^*$.

6.16 Remark: (1) The function values for Ξ_0 can also be achieved by *local* inverse distance weighting of nearby sites instead of just taking the initial value, at least in regions where the sampling is comparably dense; as long as it is local, this is also comparably efficient to achieve, either by calculation of intrinsic geodesic distance to only nearby points, or even by calculation of the Euclidean distance to such nearby points. In particular, this approach can be used to reduce noise in function evaluations locally.

(2) One could implement different and additional hierarchy levels of splines and sites to resemble further nonuniformness or irregularity in the data, or to deal with local deviations in the error.

(3) The thinning can be performed even by very simple algorithms, like iteratively removing one of the points where the intrinsic separation distance

$$q_\Xi^{\mathbb{M}} := \min_{\xi_1, \xi_2 \in \Xi} d_{\mathbb{M}}(\xi_1, \xi_2),$$

or even the extrinsic separation distance g_Ξ is attained — an idea suggested in [66], where also some additional tuning is proposed for the Euclidean case.

We exemplify the effect of the proposed method again by the parameterisation of the Stanford bunny over the pumpkin. This time, we suppose that our sampling contains a significant hole, leaving us without reasonable information on the rear side of the bunny (depicted in the first picture of Fig. 6.20).

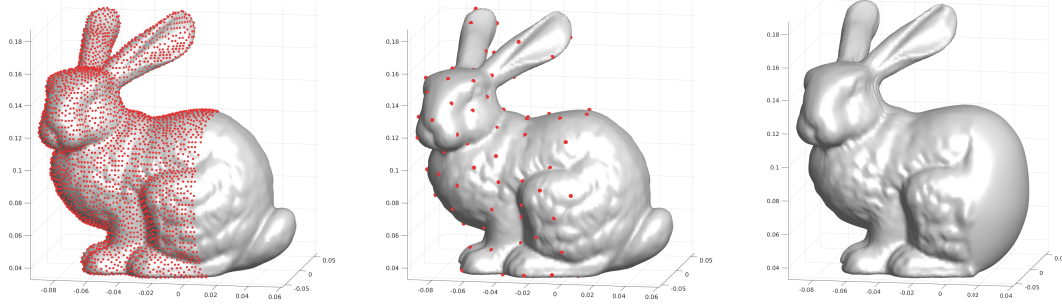


Figure 6.20: *First picture: All sampled sites displayed over the model. Note the significant lack at the rear side of the bunny. Second picture: Remaining sites after thinning substantially. Third picture: Bilevel reconstruction of bunny. The well-sampled part is approximated well, and the part without data is satisfactory estimated or extrapolated.*

Like in the previous situations, a direct approximation is again doomed to failure, as it lacks any reasonable information on the ill-sampled part of the ESM. So as before, our approach seems fully justified.

We then thin the initial 5589 sites accordingly to 120 sparse sites (depicted in the second picture of Fig. 6.20), to which we can apply extrapolation with cells for $h = 0.125$. Unfortunately, while this choice for h is more than suitable for a reasonable solution in the first hierarchy level, it turned out to be insufficient for the second level, where the two-stage approach is applied. There, we use $h = 0.03125$ instead. Luckily, this causes no true harm, as the splines of $h = 0.125$ are also contained in the space of splines for $h = 0.03125$ if the cells are suitably aligned, so we can still obtain a combined overall solution in terms of a single spline function. Details on the relation between different hierarchy levels of splines can be found in [74].

Chapter 7

Partial Differential Equations on Embedded Submanifolds

In this chapter we are looking for approximate solutions to certain partial differential equations. As the reader might already guess, we will apply the ambient penalty approximation of minima to some specific energy functionals therein. Our focus will be set on compact ESMs within this chapter, and we are only briefly commenting on situations with boundary. Furthermore, we will concentrate on essentially just two model equations that correspond to some of the previously introduced energy functionals; we leave the investigation of more general elliptical partial differential equations with all matters of well-posedness, applicability of our concepts and the like for the future, as it would lead to far here.

7.1 Elliptic Problems on Closed Submanifolds

In this section, we are going to present promising results for approximation of solutions of some model partial differential equations. As the previous chapters imply, we will concentrate on equations of the form

$$\Delta_M f - \lambda f = g$$

for some $\lambda \geq 0$ on compact ESMs — so there is no boundary, and thus there are no boundary conditions either. In the case $\lambda = 0$ however, the problem requires additional side conditions, because the kernel of Δ_M contains the constant functions; so we have to demand a single point and a function value to be fixed.

In any case, this equation gives rise to the energies

$$\mathbb{E}_\Delta^\lambda(f) := \int_M (\Delta_M f - \lambda f)^2 \quad \text{and} \quad \mathbb{E}_\Delta^\Xi(f) := \int_M (\Delta_M f)^2 + \sum_{\xi \in \Xi} (f(\xi))^2$$

introduced in section 4.3. Consequently, they also imply tangent directional versions $\mathbb{E}_{\Delta,\lambda}^\top$ and $\mathbb{E}_{\Delta,\Xi}^\top$, and corresponding ambient penalty approximation functionals. As we have seen in the respective section 4.3, we can directly include the right hand side of the equation and obtain a residual minimisation problem suitable for application of the results in Section 5.3. So we introduce the residual functional

$$R_{\Delta,M}^{\lambda,g}(S) := \int_M (\Delta_M S - \lambda S - g)^2.$$

If $\lambda > 0$ and the equation has unique solution $f^* \in H^2(M)$, we obtain APA functional

$$P_{\Delta,M}^{\lambda,g}(S, \sigma_M, \sigma_C) := R_{\Delta,M}^{\lambda,g}(S) + h^{-\sigma_M} N_M^\nabla(S) + h^{-\sigma_C} N_C^\nabla(S).$$

In case $\lambda = 0$ for arbitrary $\xi \in M$ and corresponding function value $\gamma_\xi \in \mathbb{R}$ we obtain correspondingly the two functionals

$$\begin{aligned} P_{\Delta,M}^{\Xi,g}(S, \sigma_M, \sigma_C, \sigma_\xi) &:= R_{\Delta,M}^{0,g}(S) + h^{-\sigma_\Xi} (S(\xi) - \gamma_\xi)^2 + h^{-\sigma_M} N_M^\nabla(S) + h^{-\sigma_C} N_C^\nabla(S), \\ P_{\Delta,M}^g(S, \sigma_M, \sigma_C) &:= R_{\Delta,M}^{0,g}(S) + h^{-\sigma_M} N_M^\nabla(S) + h^{-\sigma_C} N_C^\nabla(S). \end{aligned}$$

The last functional requires again a strict interpolation constraint $S(\xi) = \gamma_\xi$ to reduce the kernel from all constant functions to the zero function alone.

The exact convergence rate we can hope for depends on the actual regularity of the solution to the PDE. In our examples, we will always rely on smooth functions and therefore can presume the achievable constants β_1, β_2 in the results of Section 5.3 to be effectively optimal. That is, we can insert the convergence results for ambient B-splines of Theorem 3.29, Corollary 3.33 and the respective results on normal derivatives, so Corollaries 3.37 and 3.39. For splines of order $m \geq 4$ we can then expect that there is a family $(s_h^*)_{h < h_0}$ of restrictions of splines $(S_h^*)_{h < h_0}$

$$\begin{aligned} \|s_h^* - f^*\|_{H^2(M)}^2 &\leq c h^{2(m-2)} \|f^*\|_{H^m(M)}^2 \\ \|T_M(\nabla_N S_h^*)\|_{L_2(M)}^2 &\leq c h^{2(m-1)} \|f^*\|_{H^m(M)}^2 \end{aligned}$$

and thus $\beta_2 = 2(m-2) = 2m-4$ and $\beta_1 = 2(m-1) = 2m-2$ in case of surfaces in \mathbb{R}^3 and curves in \mathbb{R}^2 . Inserting this in the results of Theorem 5.9 for the APA convergence statement on residuals in the case without a side condition penalty, we achieve $\alpha = \min\{2m-4, 2m-2-\sigma\}$, whereby an upper bound for σ is 2.

In our first examples, we present the effects in the curve case for $\sigma_M = 1, \sigma_C = 1$ and $\sigma_M = 1.5, \sigma_C = 0.5$. These examples are obtained by considering the equations

$\Delta_{\mathbb{M}}f - 1f = g_1$, $\Delta_{\mathbb{M}}f - 2f = g_2$ and $\Delta_{\mathbb{M}}f - 4f = g_3$ on the three curves depicted in Fig. 7.1 in the first row, where g_1 is obtained for curve length L (depending on the respective curve, of course) by insertion of the function

$$f_1 : t \mapsto \cos(5/L \cdot (2\pi)t), \quad t \in [0, L[$$

in the equation. Similarly, g_2, g_3 are obtained by insertion of

$$f_2 : t \mapsto \cos(4/L \cdot (2\pi)t), \quad t \in [0, L[.$$

The experimental convergence rates are also presented there, right below the respective curves. We obtain roughly the expected convergence orders for spline orders $m = 4, 5, 6$. However, at least the latter is running into some saturation. This can presumably be attributed to the unfavorable ratio of stabilising cells versus support sizes in that case. We also see the convergence behaviour of the L_2 error there, and once again cannot really draw a conclusion on a certain convergence order, except that it is obviously controlled by the energy error.

In these examples, we also see that while different penalty exponents produce the expected convergence, the penalty on the space in particular should be chosen lower if possible: This can be expected to have a positive effect on the results, although stability issues may arise if in particular $\sigma_C = 0$ is chosen.

As pointed out before, any choice for $\sigma_{\mathbb{M}}$ and σ_C between 0 and 2 is valid and has no effect on the convergence at least theoretically. However, particularly if the space penalty exponent σ_C was small, like $\sigma_C = 0$, then the stability could suffer. And if it was (too) high, we could run into saturation rapidly at least for higher spline orders. There, the normal directional derivative can become dominant in the minimisation problem at least from a numerical point of view. That does usually rarely occur for cubics however, indicating further that the problem has numerical, not theoretical reasons. On the other hand, exponent $\sigma_C = 2$ in the space penalty would consume a lot of degrees of freedom also in the cubic case, and therefore have a negative effect on the actual quality — it was still reasonable, but better choices yielded better results. Of course, one can also use different penalties σ_C in space and $\sigma_{\mathbb{M}}$ on the ESM again. If we take this into account, then the results for $0 \leq \sigma_C \leq 1$ and $1 \leq \sigma_{\mathbb{M}} \leq 2$ were roughly comparable and all quite satisfactory: The exact outcome would depend on the ESM geometry, and a good choice could still mean a gain of one or two orders of magnitude in the L_2 error, while the energy error was quite stable under such modifications and only mildly affected.

The expected convergence order in the energy norm as the square root of $\mathcal{E}_{\Delta}^{\lambda}(f)$ is then the optimal h^{m-2} , and we already know that this norm is equivalent to the standard norm of $H^2(\mathbb{M})$. Similar to $P_{\Delta}^{\lambda,g}$, also the other functionals can be handled.

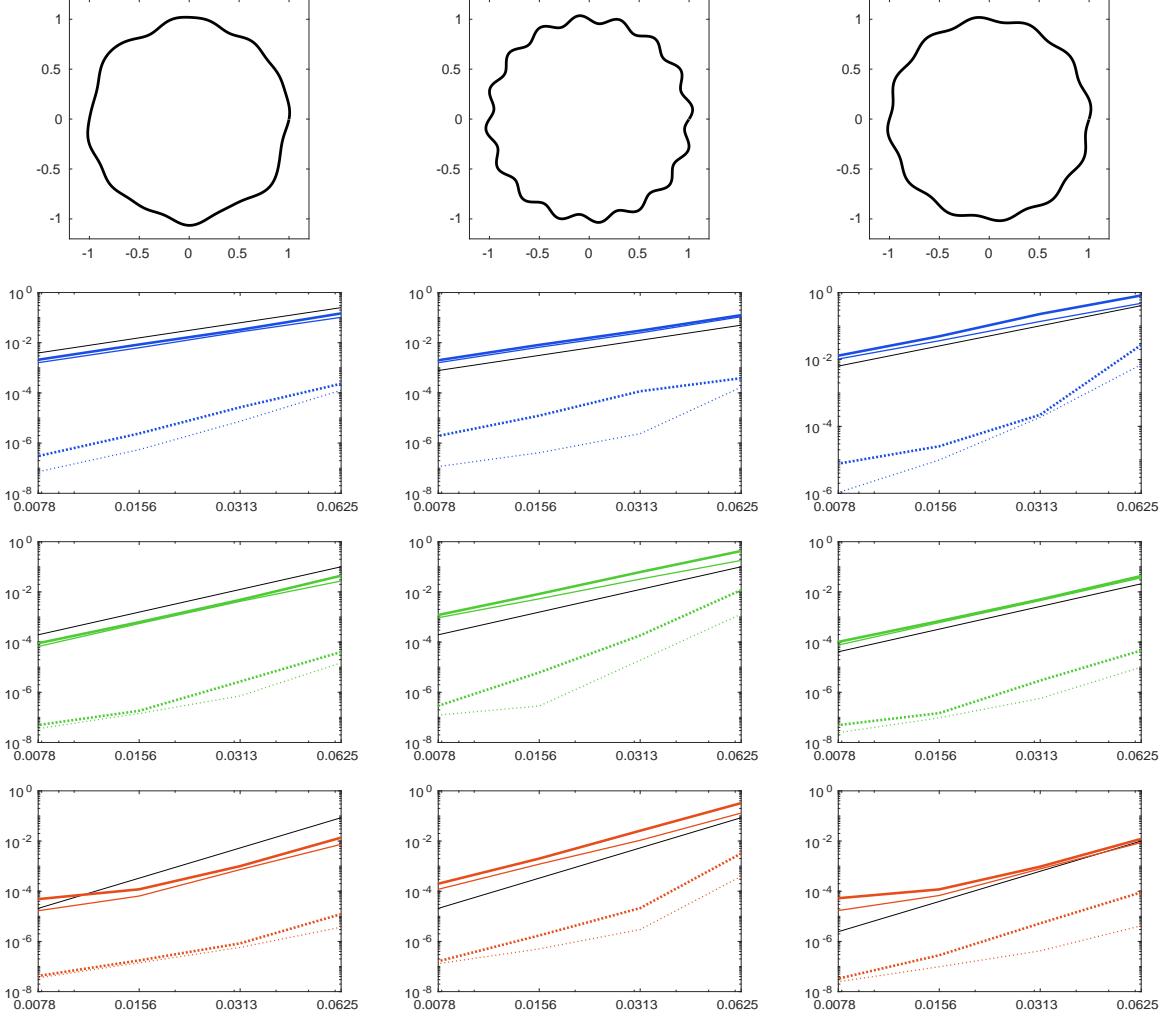


Figure 7.1: Example curves and corresponding convergence orders: Convergence orders for examples (blue: bicubics, green: biquartics, orange: biquintics) with penalty exponents $\sigma_M = 1, \sigma_C = 1$ (thicker) and $\sigma_M = 1.5, \sigma_C = 0.5$ (thinner). — energy error (colored: approximation, black: references h^2, h^3, h^4), L_2 -error (colored: approximation), all deduced for linear integral approximation with about $600[1/h]$ points. First row: Insertion of f_1 with $\lambda = 4$. Second row: Insertion of f_2 with $\lambda = 2$. Third row: Insertion of f_2 with $\lambda = 1$.

We will now turn to further examples presented in Fig. 7.2. These examples feature several further solutions f^* , one that is less fluctuous and one that is more fluctuous than the ones before. Furthermore, we also consider curves with more intricate geometry and with less intricate geometry, and with geometries that have regular and irregular deformations. Similar to the previous examples, we now concentrate just on the equation $\Delta_M f - f = \tilde{g}_j$ for $j = 1, 2, 3$. These g_j are obtained by insertion of functions f_2, f_3, f_4 into the equation, for f_2 as above and the functions

$$f_3 : t \mapsto \cos(9/L \cdot (2\pi)t) + \sin(3/L \cdot (2\pi)t), \quad f_4 : t \mapsto \cos(1/L \cdot (2\pi)t) + \sin(1/L \cdot (2\pi)t).$$

In our tests, we found the expected convergence behaviour verified again for all

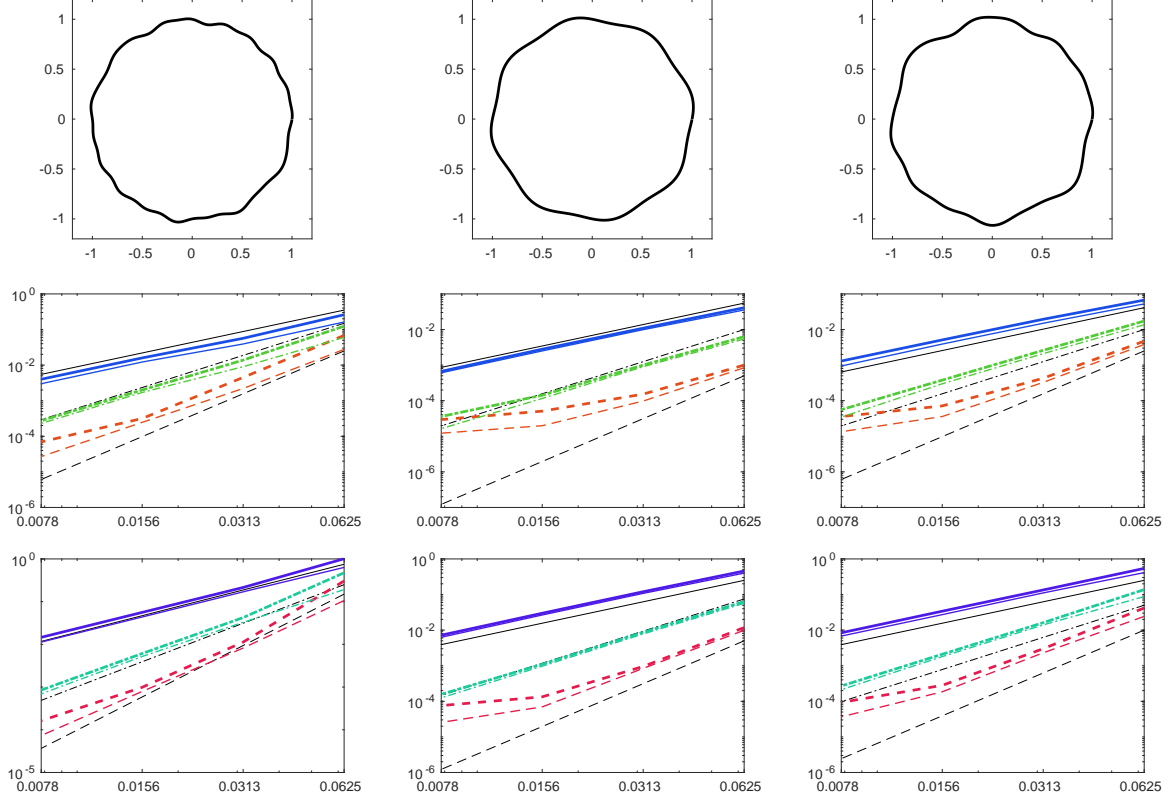


Figure 7.2: Example curves and corresponding convergence orders. Approximation of f_2 (second row) and f_3 (third row) with orders $m = 4$ (blue/violet, solid), $m = 5$ (green/teal, dot-dashed) and $m = 6$ (orange/crimson, dashed). References h^2 (solid), h^3 (dot-dashed) and h^4 (dashed) all black.

spline orders, with a saturation at least in the quintic case around some 10^{-4} or 10^{-5} . Again, we have also convergence of L_2 error until some saturation about two to three powers smaller, so at about 10^{-7} or 10^{-8} . The saturation effect occurred in particular for quintic splines, as the plots show — where of course these gave also the best approximations of the three. We attribute this effect particularly to the fact that for quintic splines the conditioning of the system suffered most from the increased ratio between support size and cell size. So for increasing order the stabilizing effect of the “cell penalty” gets more and more lost.

That this effect is indeed some kind of saturation is also supported by the plots and results presented in Fig. 7.3, as there we have more intricate geometry, and thus higher errors in the beginning, leading to the expected convergence behaviour until at least an energy error of 10^{-4} or less. There, it seems also to have little impact which of the penalty exponents we choose, so we just depict the results for overall $\sigma = 1$. Note in particular that even for this intricate geometry, the error of order zero decreases rapidly to a satisfactory value in all cases.

As the final example for curves, we will also investigate the case $\lambda = 0$. As mentioned before, this case requires a special treatment, as the functional implied by

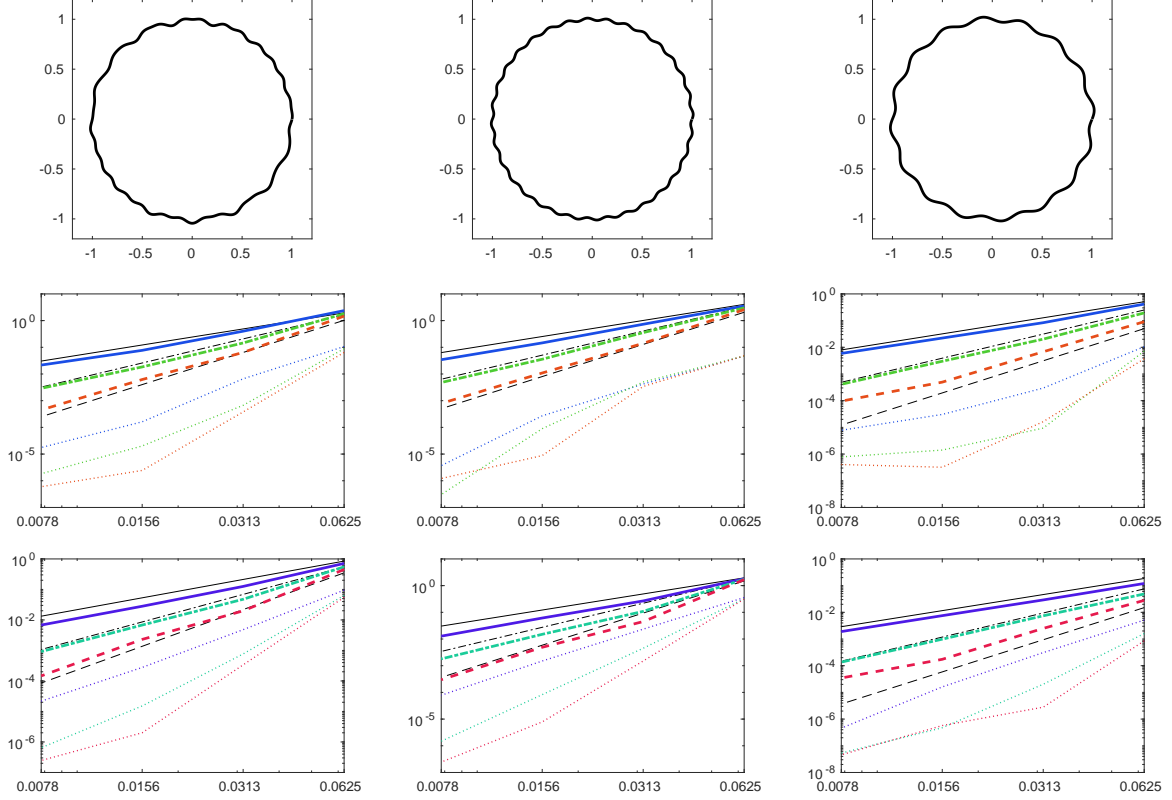


Figure 7.3: Example curves and corresponding convergence orders. Approximation of f_2 (second row) and f_4 (third row) with orders $m = 4$ (blue/violet, solid), $m = 5$ (green/teal, dot-dashed) and $m = 6$ (orange/crimson, dashed). References h^2 (solid), h^3 (dot-dashed) and h^4 (dashed) all black. All plots feature also the respective rms error of order zero, dotted in the respective color.

the equation itself does only give a positive semidefinite quadratic functional, because Δ_T and Δ_M both map constants to zero. Consequently, we have to fix at least one function value or have to enforce this function value by a penalty of the form

$$h^{-\sigma_{\Xi}} \sum_{\xi \in \Xi} (S(\xi) - v_{\xi})^2.$$

Both mean no harm here. In the first case, we still retain all relevant properties for our choices of β_1, β_2 except for “ $-\varepsilon$ ”, and in the second we just have to make the right choice for σ_{Ξ} : For functions like those considered here, we can expect convergence of function values to be of order h^m as well — we have stated in Remark 3.20 that in this case we can expect optimal convergence in the maximum norm, too. So we deduce that $\beta_{co} = 2m$ and we can choose $\sigma_{co} \leq m$. But since we expect that we loose nothing in the convergence if the interpolation is strict, we would actually expect any choice of σ_{co} to work out. And indeed, for tests with different values from $\sigma_{co} \in \{2, 3, 4\}$ we find no relevant impact on the convergence and an error of the function value in the specified point is close to machine precision.

We have depicted the results for insertion of functions f_2 and f_4 into the equation

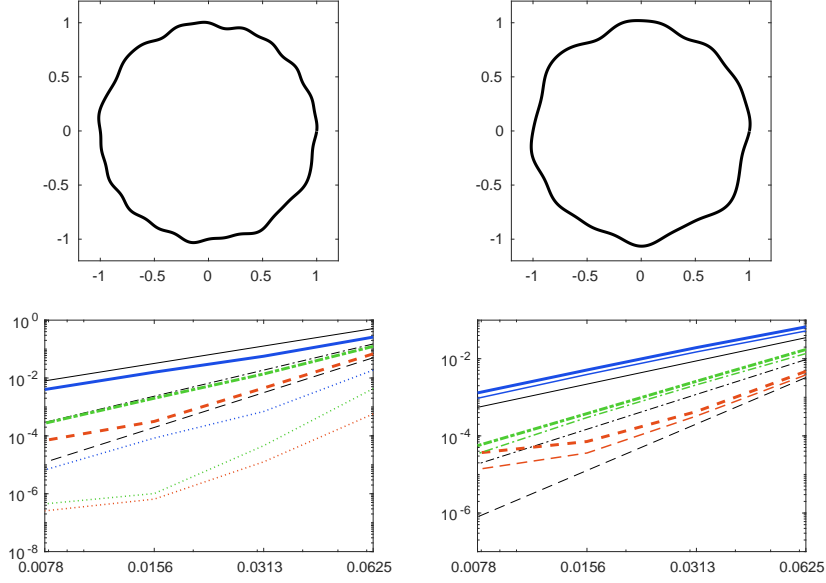


Figure 7.4: Example curves and corresponding convergence orders for approximation of f_2 in case $\lambda = 0$: Convergence orders for examples: — Laplacian energy error (colored: approximations by orders 4, 5, 6 (blue, green, orange), black: references h^2, h^3 , in the right picture also thinner for $\sigma_M = 1.5, \sigma_C = 0.5$). In the left picture also: - - - L_2 error for approximations by orders 4, 5, 6 (blue, green, orange), all deduced for linear integral approximation with about $600[1/h]$ points.

Fig. 7.4. For the interpolation penalty variant, we used a penalty exponent $\sigma_{\Xi} = 3$ here, which effectively lead to interpolation as well, with a function value error of about 10^{-15} . Also, the resulting functions and errors for strict interpolation and interpolation penalty were effectively coincident. So we present only one version in the plots. They show little to no deviations to the respective plots for the case of $\lambda = 1$ depicted in the preceding figures: Again, the convergence orders are about what we have expected, and also with pleasant values of order zero rms.

Now it is once more time to switch to surfaces. We will investigate the surfaces depicted in Fig. 7.5. These (smooth) surfaces are again required to be discretised as a list of triangles with normals assigned to each vertex, so that we can apply approximate piecewise linear integration.

In our tests, we used the insertion of the two functions $f_{3,1}$ and $f_{3,2}$ into $\Delta_M f - f$ to create our examples. The first function is given as $f_{3,1} = \mathbb{T}_M F_{3,1}$ for

$$F_{3,1}(x, y, z) := \frac{3}{4}e^{-(9x-2)^2/4-(9y-2)^2/4} + \frac{3}{4}e^{-(9x+1)^2/49-(9y+1)/10} \\ + \frac{1}{2}e^{-(9x-7)^2/4-(9y-3)^2} - \frac{1}{5}e^{-(9x-4)^2-(9y-7)^2} \\ + \sin(x+y)\exp(xy)\cos(4y+z).$$

In the same way, the second function is given as $f_{3,2} = \mathbb{T}_M F_{3,2}$ for

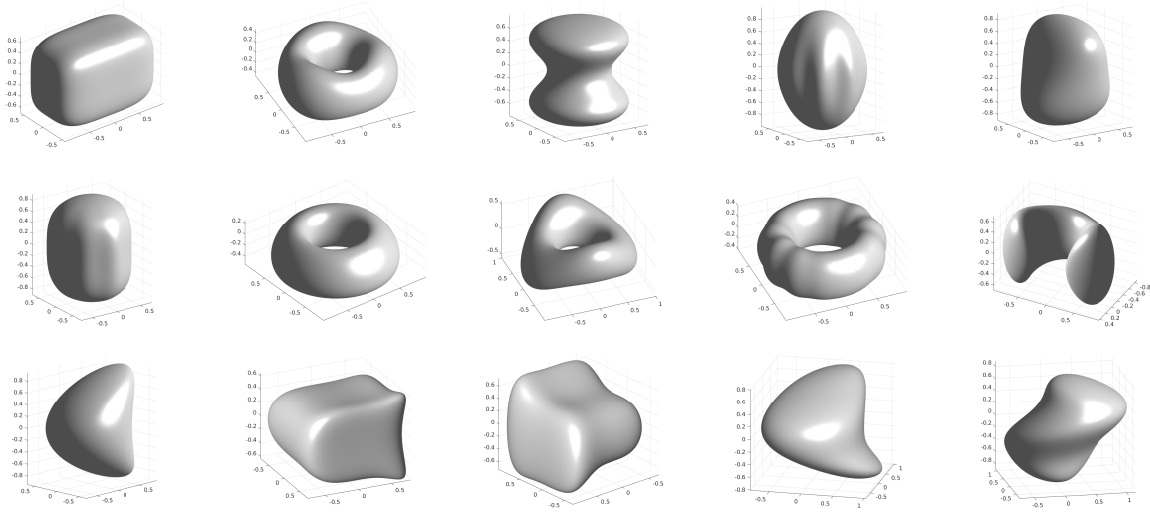


Figure 7.5: Example surfaces.

$$\begin{aligned}
 F_{3,2}(x, y, z) := & \frac{1}{4}e^{-(9x-2)^2/4-(9y-2)^2/4} + \frac{1}{4}e^{-(9x+1)^2/49-(9y+1)/10} \\
 & + \frac{3}{4}e^{-(9x-7)^2/4-(9y-3)^2} - \frac{1}{4}e^{-(9x-4)^2-(9y-7)^2} \\
 & + \cos(x+y) \log(x^2y^2+1) \sin(4y^2+z).
 \end{aligned}$$

Again, we find the expected rates of convergence verified for both tricubics and triquartics: The residual, and consequently also the energy, converges at the expected rate of convergence, h^2 or h^3 . And as before, the L_2 -rms error is also quite satisfactory, though not decreasing as regularly as the residual error. The results are depicted in the subsequently following figures 7.6, 7.7 and 7.8.

7.1 Remark: (1) Unfortunately, triquintic splines can suffer from an early saturation and also the creation of corresponding systems would become increasingly costly. Thus we did not include them in the convergence analysis here any further. (2) The saturation of the L_2 -rms error can probably be attributed to one of the following effects:

- The numerical integration might be not exact enough to represent the zero order part of the functional sufficiently accurate, although it was sufficient for the energy.
- The used penalty exponents make the respective part of the APA functional numerically dominant compared to the zero order part of the functional.
- The zero order part of the functional is by orders of magnitude smaller than the part of first and particularly of second order. This means that when the corresponding system becomes large and the numerical errors start to accumulate, the zero order part is the first to fall behind.

- The discretisation of M itself is not accurate enough, as the triangulation algorithm of Matlab employed is not necessarily giving exact vertices on M — deviations by about 10^{-5} to 10^{-8} could easily occur.

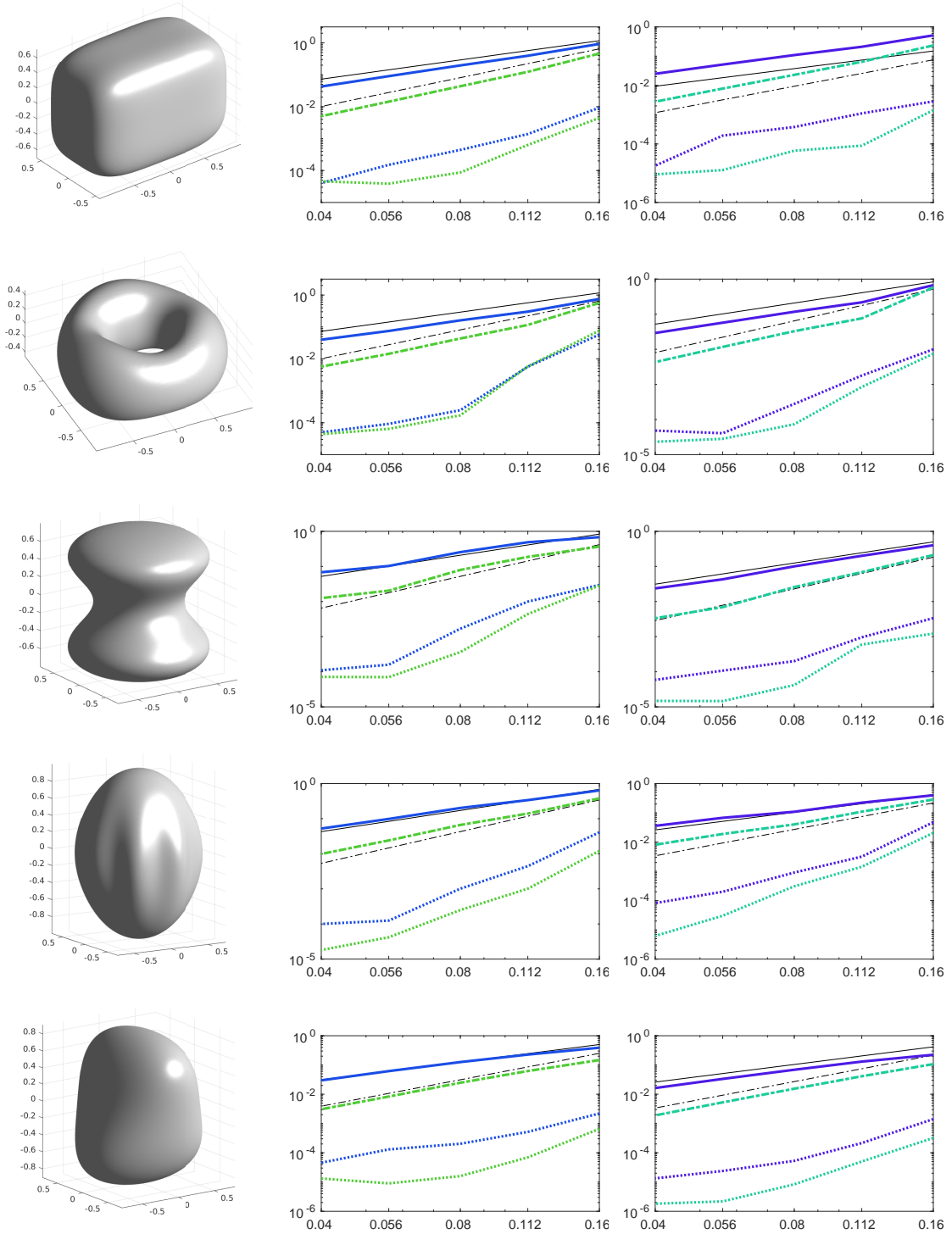


Figure 7.6: Surfaces and experimental convergence for energy (so second order) and zeroth order. The L_2 error of order zero (normalised via division by surface area) is dotted, and the (normalised) error for the energy is solid (cubics) and dash-dotted (quartics). Results for cubics are blue/violet, results for quartics are green/teal. All used a penalty exponent $\sigma = 1$.

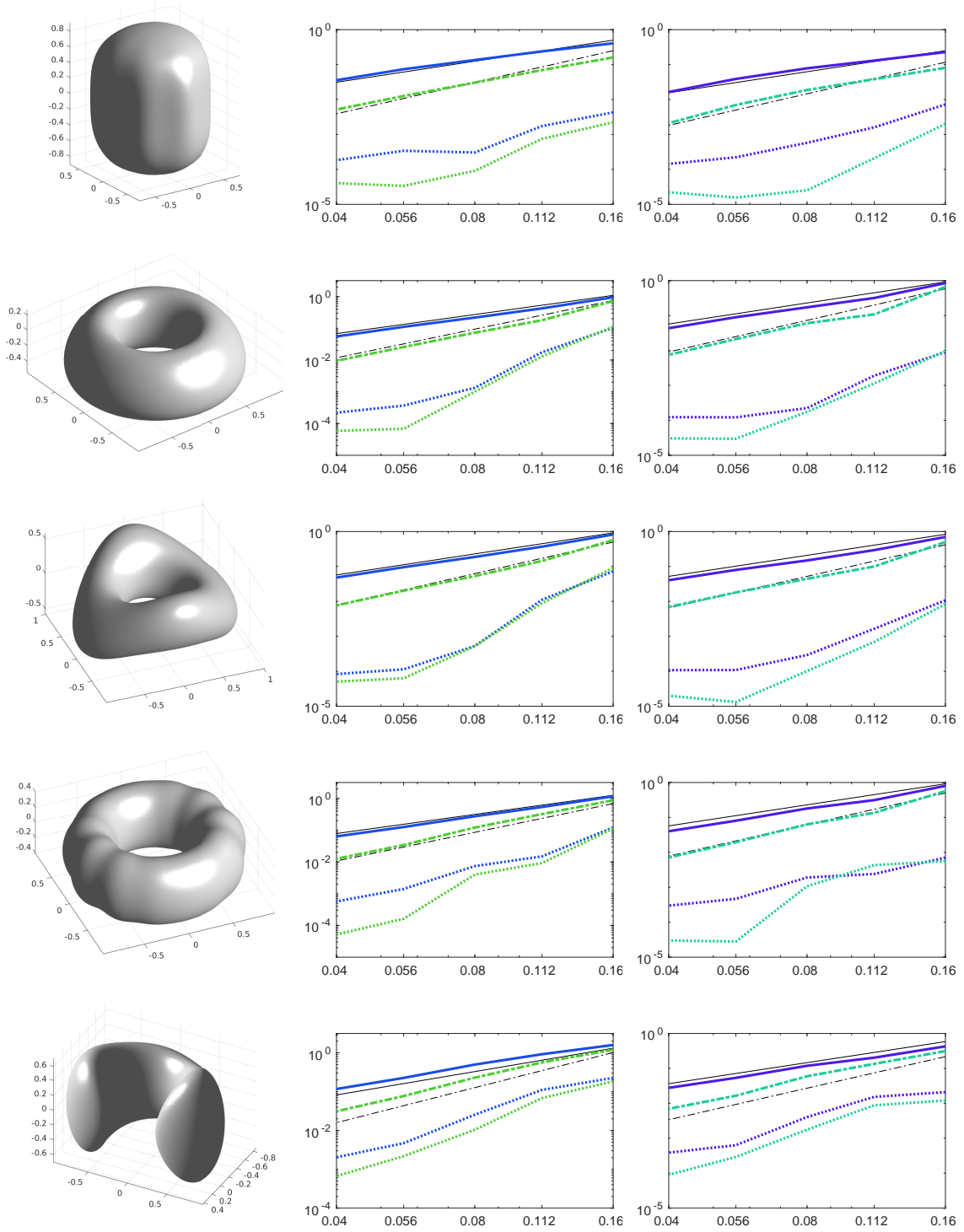


Figure 7.7: Further surfaces and experimental convergence for energy (so second order) and zeroth order error. As before, the (normalised) error of order zero is dotted, and the (normalised) error for the energy is solid (cubics) and dash-dotted (quartics). Results for cubics are blue/violet, results for quartics are green/teal. All used a penalty exponent $\sigma = 1$.

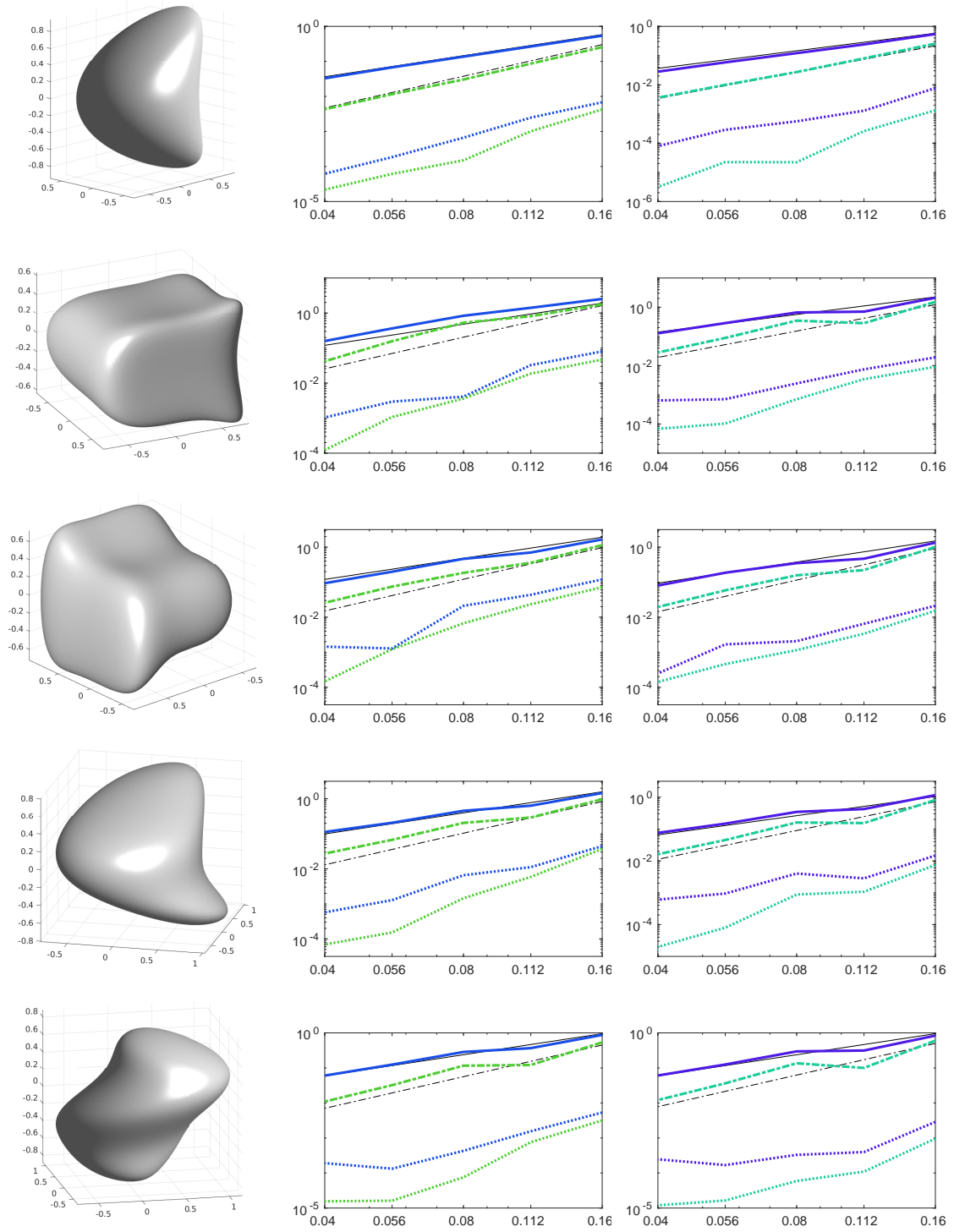


Figure 7.8: Further surfaces and experimental convergence for energy (so second order) and zeroth order error. As before, the (normalised) error of order zero is dotted, and the (normalised) error for the energy is solid (cubics) and dash-dotted (quartics). Results for cubics are blue/violet, results for quartics are green/teal. All used a penalty exponent $\sigma = 1$.

7.2 Ideas for Open Subdomains of Submanifolds

In contrast to the case of compact ESMs, partial differential equations of the same type on open ESMs (or subdomains of ESMs) require additional boundary conditions to ensure unique solvability, for example an additional $f = 0$ on the boundary Γ_0 of subdomain $M_0 \Subset M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$. In this case, the square root of $\mathcal{E}_\Delta^\lambda$ is no longer known to be an equivalent norm on $H^2(M_0)$. However, we still retain what we discussed in the end of section 5.3: We can include the boundary conditions in the penalty and create a penalty functional of the form

$$P_{\Delta, M_0}^{\lambda, g}(S, \sigma_M, \sigma_C, \sigma_{\text{co}}) := R_{\Delta, M_0}^{\lambda, g}(S) + h^{-\sigma_M} N_M^\nabla(S, M_0) + h^{-\sigma_C} N_C^\nabla(S, M_0) + h^{-\sigma_{\text{co}}} \int_{\Gamma_0} |S|^2.$$

We can deduce at least residual convergence that corresponds to the energy norm convergence of the last section: The results of Corollary 5.11 give us convergence of the residual $\mathcal{E}_\Delta^\lambda(s_h - f^*)$ of order h^α for $\alpha = \min\{(\beta_1 + \beta_2)/2, \beta_2, \beta_1 - \sigma, \beta_{\text{co}} - \sigma_{\text{co}}\}$. While we can simply reuse the values of β_1, β_2, σ from the previous situation without boundary, we will have to make some further brief considerations for β_{co} and σ_{co} : By the (integer) trace theorem, we can expect that for $s = S|_{M_0}$

$$\int_{\Gamma_0} |S|^2 = \int_{\Gamma_0} |s - f^*|^2 \leq \|s - f^*\|_{H^1(M_0)}^2,$$

and therefore we can directly conclude that we can expect at least $\beta_{\text{co}} = \beta_2 + 2$ and thus see that we can choose at least $\sigma_{\text{co}} = 2$. In fact we would expect even $\beta_{\text{co}} > \beta_2 + 3 - \varepsilon$ for any $\varepsilon > 0$, but we found $\sigma_{\text{co}} = 2$ sufficient in our tests.

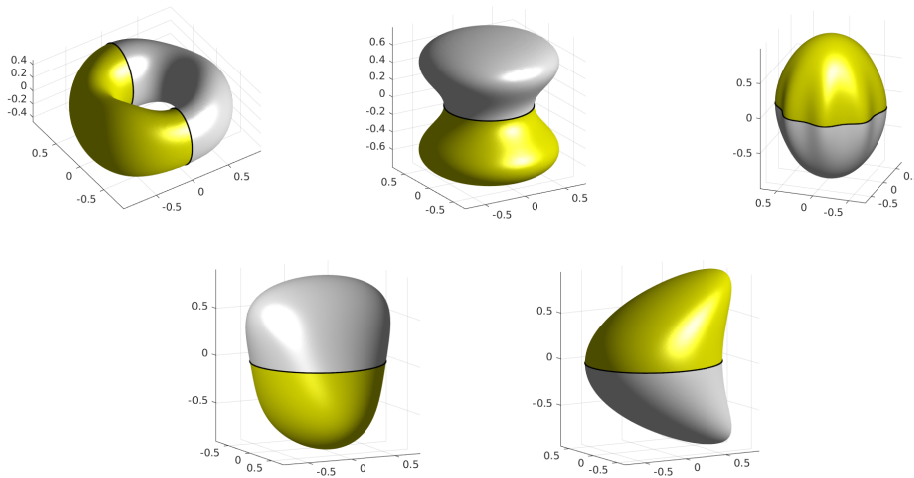


Figure 7.9: Example surfaces cut along the section curves depicted in black. This decomposes the surfaces in two parts, depicted in silver and yellow.

For these tests, we simply cut some of the surfaces from the previous examples in two parts — along the (x, z) -plane or (x, y) -plane. This gives us several situations of subdomains with boundary that are ESMs in $\mathbb{M}_{\text{sd}}^2(\mathbb{R}^3)$, depicted in Fig. 7.9.

Our tests can then use almost the same functions as before, we just multiply by x or z appropriately to achieve a function that itself satisfies the boundary conditions: We set therefore

$$\begin{aligned} F_{3,3}(x, y, z) &= x \cdot F_{3,1}(x, y, z), & F_{3,4}(x, y, z) &= z \cdot F_{3,1}(x, y, z), \\ F_{3,5}(x, y, z) &= x \cdot F_{3,2}(x, y, z), & F_{3,6}(x, y, z) &= z \cdot F_{3,2}(x, y, z) \end{aligned}$$

In the tests, we use as before $\lambda = 1$. We further rely once again on a penalty exponent $\sigma = 1$, and we use again a slightly enhanced set of cells, namely that whose centers have distance to M_0 less than h . Projection is performed onto the whole of M for those cells this time — or, to be more precise, on that part of M that was necessary to do so.

The results of the tests are depicted in Fig. 7.10 and Fig 7.11. There we see the expected convergence of the residual, and also convergence of the boundary values as well as a behaviour of the zeroth order error like in the case of compact surfaces. The only difference is that the residual is no longer directly equivalent to the norm of $H^2(M)$, but apart from that the results are promising.

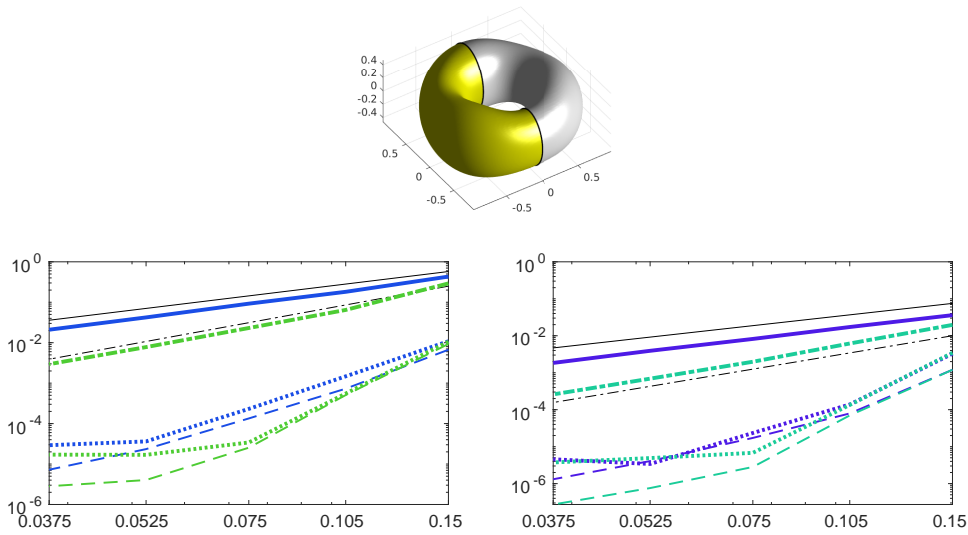


Figure 7.10: Example surfaces and practical rates of convergence for (normalised) energy error and (normalised) L_2 error. As before, the L_2 error of order zero is dotted, and the error for the energy is solid and dash-dotted, respectively. The boundary condition root mean square error is depicted dashed. Results for cubics are depicted in (blue/violet), results for quartics are depicted in (green/teal). All used a penalty exponent $\sigma = 1$. The left convergence plot is based on the silver part of the surface and approximation of function $f_{3,3}$, while the right plot is based on the golden part and insertion of $f_{3,5}$.

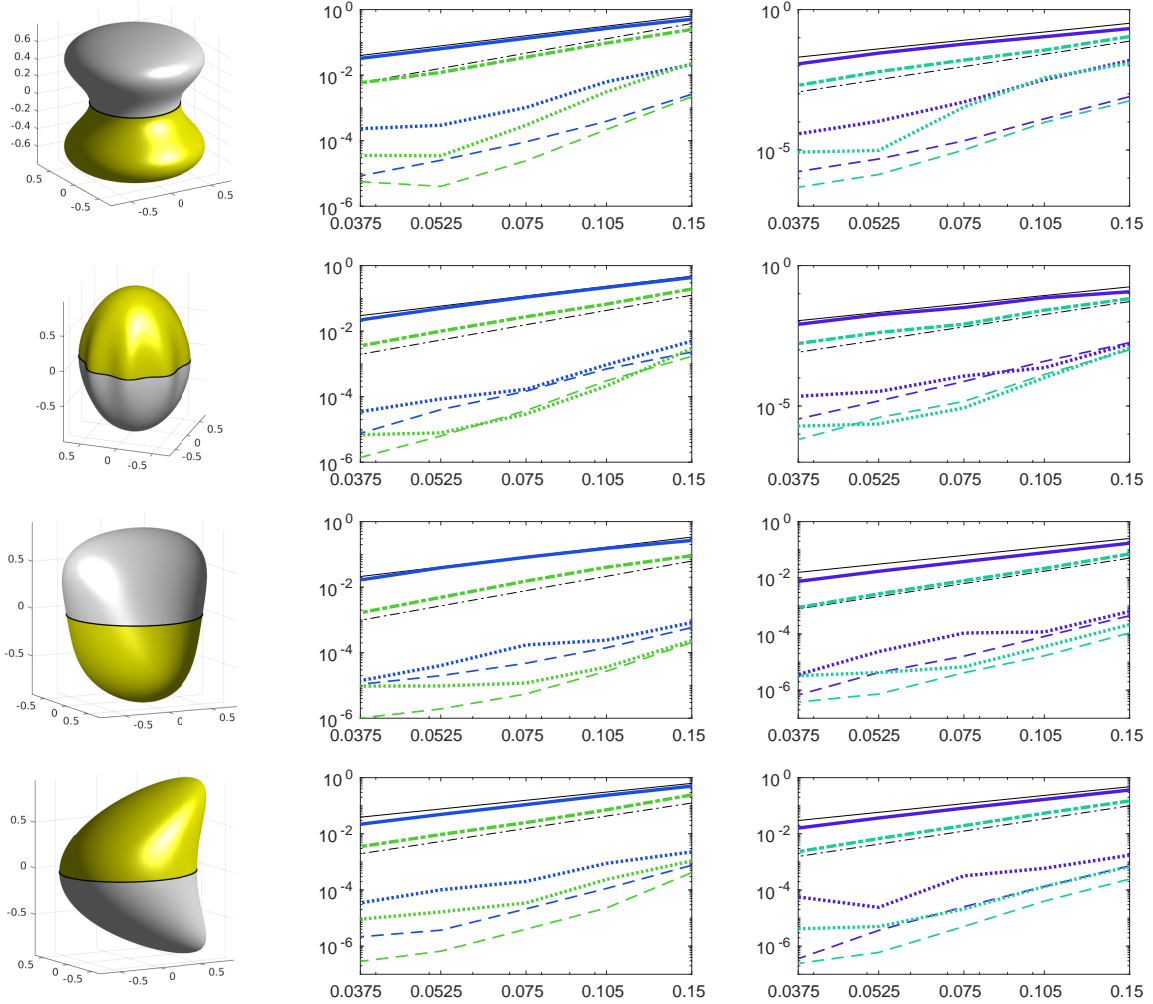


Figure 7.11: Example surfaces and practical rates of convergence for (normalised) energy error and (normalised) L_2 error as well as boundary error. As before, the L_2 error of order zero is dotted, and the error for the energy is solid and dash-dotted, respectively. The boundary condition root mean square error is depicted dashed. Results for cubics are depicted in (blue/violet), results for quartics are depicted in (green/teal). All used a penalty exponent $\sigma = 1$. The left convergence plots are based on the silver part of the surface and approximation of function $f_{3,4}$, while the right plot is based on the golden part and insertion of $f_{3,6}$.

Chapter 8

Conclusion and Prospects

In this thesis, we have presented a number of new or enhanced approaches to many approximation problems on embedded submanifolds. These include

- extended and enhanced convergence results for the ambient approximation method, which gives us optimal convergence rates for suitable Sobolev norms when applied to tensor product splines by local quasi-projections,
- convergence results for ambient approximation operators under point constraints and for *normal* derivatives,
- a thorough analysis of relations between first and second order intrinsic (tangential) and extrinsic (Euclidean) derivatives for functions on embedded submanifolds,
- an analysis of the kernel of the second order tangential derivative operator under finite interpolation constraints that transferred the concept of unisolvency to the submanifold setting,
- a general framework for the approximation of minimisers to a whole range of intrinsic second order functionals, the *augmented equivalently* E_N -*extrinsic* functionals, by the *ambient penalty approximation* (APA) method,
- specific methods for extrapolation of sparse data and for smoothing on embedded submanifolds that yield approximate functional minima via APA minimisation and provide also pleasant practical results,
- specific methods for the solution of a model PDE by APA-based residual minimisation that provide optimal convergence of the residual for both open and closed submanifolds, with the latter providing optimal convergence of a second order Sobolev norm as well.

Nonetheless, numerous extensions and further developments or deeper investigations remain open for future research:

First of all, it would be interesting to check for other approximation methods that meet the requirements of the ambient approximation method we proposed, for instance radial basis functions, moving least squares or other methods providing suitable quasi-interpolations. This could then also lead to applicability of the APA functional minimisation with these approximation methods.

In the present thesis, all submanifolds were required to be bounded. Therefore, a generalisation of all results to suitable unbounded embedded submanifolds would be interesting and increase the applicability of the concepts introduced here.

One way to overcome the unsatisfactory restrictions with respect to the submanifold dimension k when minimizing energy under fixed interpolation constraints would be to turn to higher orders for energy estimation, so to consider not the second, but possibly the third, fourth or ℓ th tangential derivative. In achieving this, one would have to prove correspondence of tangential and Euclidean derivatives of constant extensions also in this setting. And one would also have to find conditions under which a given set of points provides suitable intrinsic unisolvency.

Regarding the concept of APA minimisation in general, the conditioning of the system and in particular the impact of the "space penalty" on the stability was not investigated systematically so far, and a deeper insight might help in further improving convergence rates and actual results of the method.

Another interesting question is what happens if the underlying ESM is not (infinitely) smooth. Of significant importance in practice are in particular the cases of C^0 -, C^1 - and C^2 -submanifolds. In some brief numerical tests, it seemed that if the presented method is applied straightforwardly to such ESMs, this is desperate for the case C^0 , gives reduced convergence order for C^1 and produces effectively the same orders as in the smooth case for C^2 , but the matter definitely requires further investigation.

One major drawback of the APA approach seems to be that if the geometry is very intricate, a significant number of cells is required to resolve the geometry of the ESM suitably. To overcome this, approaches based on hierarchical splines might be beneficial, and these could also be employed in adaptive refinement for further improvement of approximation results.

Another drawback of effectively any ambient space method is apparantly what could be called the *curse of codimensionality*, in correspondence to the well-known curse of dimensionality: If the codimension increases, then the number of functions on each spline cell is, roughly speaking, some m^d , not only some m^k . That means that when the codimension is large, this can become prohibitive to reasonable application: It even plays a crucial role if a surface is embedded into \mathbb{R}^3 or in \mathbb{R}^4 , and it would be interesting to find out if there is some way to overcome this. So

one would need to determine if the number of basis functions could be reduced in that respect without losing approximation power.

An application and further investigation of the presented method for energy minimisation might also be particularly interesting in terms of statistics and machine learning: There is a huge demand for suitable fast and easy regression methods that could presumably be deduced directly from our approach, also in terms of Tikhonov regularisation — but the exact statistical properties would have to be investigated thoroughly.

Further, a detailed discussion of the actual regularity of the optimal solutions for these problems, and of achievable convergence rates, would be beneficial.

Regarding the solution of partial differential equations, it would first of all be very interesting to investigate the tangential formulations and suitable requirements for such formulation in more general elliptic equations, and subsequently also for other types of second or higher order PDE. Furthermore, convergence results in the case with boundary, convergence orders for Sobolev norms of lower orders than the energy order 2 and the inclusion of Neumann and other boundary conditions into the APA functional would be interesting. And in the case with a boundary, we could also hope to apply some kind of maximum principle to obtain a-posteriori error bounds for our approximations.

Finally, a suitable adaption of our concept of equivalently E_N -extrinsic functionals in terms of a Galerkin formulation of intrinsic PDE and a corresponding APA-related formulation seems to be a promising approach as well, as brief numerical tests imply.

Chapter 9

Appendix

9.1 An Atlas for Embedded Submanifolds

We are now going to provide a full construction scheme for a suitable inverse atlas that meets all the requirements we have for our inverse atlases on ESMs.

9.1.1 The Exponential Map

The first concept for the ESM itself we will require and use is that of the *exponential map* of an ESM. We present it along with some basic results on how to employ this map for the construction of a useful inverse atlas to an ESM (cf. [9, §3], [13, Prop. 88]):

9.1 Definition Let $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$, $x \in M$ and $T_x M \cong \mathbb{R}^k$ the tangent space in x . Then for some suitably small open ball $B_{r_x}^k(0) \in \mathbb{R}^k \cong T_x M$ the *exponential map* $\exp_{x,M} : B_{r_x}^k(0) \subseteq \mathbb{R}^k \rightarrow M$ is defined by

$$\exp_{x,M}(z) := \begin{cases} x & \text{if } z = 0 \\ \gamma_{x,z}(\|z\|_2) & \text{otherwise} \end{cases},$$

where $\gamma_{x,z}$ is the uniquely defined arc-length parameterised geodesic that contains x and has direction v_z for some suitable identification v_z in $T_x M$ of z in \mathbb{R}^k .

9.2 Proposition For a smooth $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$, the exponential map \exp_x is a smooth diffeomorphism in a suitably small ball $B_{r_x}^k(0)$ for any $x \in M$ and $r_x \in]0, \infty]$ called injectivity radius. If M is topologically complete, then $r_x = r(x)$ depends continuously on x .

We can also define a distance function $d_M(\cdot, \cdot)$ on M : If we consider curves $\gamma : [0, 1] \rightarrow M$, then we obtain a distance function on M as

$$d_M(x, z) := \inf \left\{ \int_{[0,1]} \|\gamma'\|_2 : \gamma(0) = x, \gamma(1) = z \right\}.$$

Because the relative closure of any nonclosed M is compact in our case as it is a subdomain of a compact ESM, this is well defined and finite even in that case. And if additionally $z \in \exp(B_{r_x}(0))$, then it is well known that the respective curve realising the distance is a geodesic from x to z . Even better, the following holds:

9.3 Corollary *Within $\exp(B_{r_x}(0))$, the squared distance function $d_M(x, z)^2$ is as smooth as M .*

Proof: This is clear because of the smoothness of the exponential map and the one-to-one correspondence between Euclidean distance of $\exp_x^{-1}(z)$ to 0 and the intrinsic distance of z to x that is directly implied by the definition. \square

9.1.2 The Construction of an Atlas

First of all, we can now find a finite inverse atlas of a compact ESM that is made up just of balls as parameter spaces and exponential maps as parameterisations: The exponential map $\exp_{x,M}$ of M is injective in a radius $r(x)$ around the origin, and that radius is a continuous function of x . So by compactness of M there must be a minimal $r^* > 0$ over all of M . Thus we can take the exponential map and any $0 < r < r^*$ to obtain an open cover of M by considering the images of the open balls $B_r^k(0)$ under $\exp_{x,M}$ to all $x \in M$. By compactness, there is a finite subcover, and $\exp_{x,M}$ for arbitrary $x \in M$ is C -bounded on any closed ball $B_r^k(0)$.

9.4 Remark: If we want to have fixed functions T, N that map any point $z \in B_r^k(0)$ to an orthonormal frame of the tangent or normal space in $\exp_{x,M}(z)$, then we can easily achieve this by application of Gram-Schmidt orthonormalisation. To make these functions well-defined on all of $B_r^k(0)$, we can be required to reduce r further, but by compactness we can still find a sufficiently small $r > 0$ that works on all of M and gives a finite subcover.

This construction would suffice for our desired inverse atlas if we have only compact ESMs. But as we do have subdomains with boundary as an option, we have to invest considerably more work. So let us have a closer look at the parameterisations of our ESMs. To achieve our goal of a finite inverse atlas where any inverse of a chart is suitably C -bounded and any parameter space is a Lipschitz domain also in the case with boundary, we will need some auxiliary results that are also interesting in their own right:

9.5 Theorem — Intrinsic Tubular Neighbourhood Theorem —

Let $\Gamma \in \mathbb{M}_{cp}^{k-1}(\mathbb{R}^d) \cap \mathbb{M}_{bd}^{k-1}(M)$ be orientable within M for $M \in \mathbb{M}_{cp}^k(\mathbb{R}^d)$. Let $\nu :$

$\Gamma \rightarrow \text{TM}$ be a smooth unit vector field that is normal to Γ . Then there is $\delta > 0$ such that on the set $\Gamma \times]-\delta, \delta[$ the map $\psi_{\Gamma, \text{M}}$ is injective, where

$$\psi_{\Gamma, \text{M}} : (x, t) \mapsto \exp_{x, \text{M}}(t \cdot \nu(x)).$$

The image of this set under the respective map is the intrinsic tubular neighbourhood $U_\delta^{\text{M}}(\Gamma)$.

Proof: We note that by the required orientability of Γ it is easily verified that such normal field exists always. Almost copying the ideas of [44], we then note that the Jacobian of $\psi_{\Gamma, \text{M}}$ is clearly nonsingular in any $(x, 0)$, and that map is smooth: M is a smooth ESM, \exp is smooth and ν as well. Consequently, the inverse function theorem and the compactness of Γ give the existence of a suitable $\delta > 0$. \square

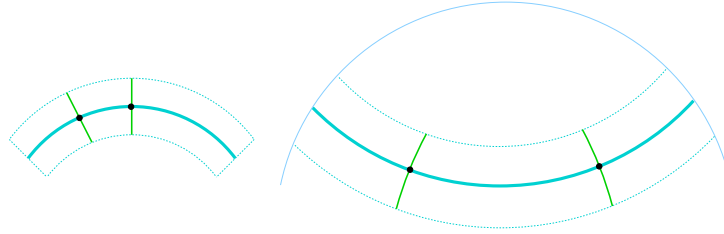


Figure 9.1: Depicted on the left is a tubular neighbourhood of a curve in \mathbb{R}^2 with $B_\epsilon^{\text{N}}(\cdot)$ to two points. Depicted on the right is an intrinsic tubular neighbourhood of a curve in \mathbb{S}^2 , again with orbits of $\exp_{\text{M}, x}(t \cdot \nu(x))$ for fixed x and varying t .

The following theorem now gives us the existence of an inverse atlas with Lipschitz parameter spaces and C -bounded parameterisations that will lead to our “inverse atlas of choice” for this thesis:

9.6 Theorem *If $\text{M} \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$, then there is a finite inverse atlas $\mathbb{A}_{\text{M}} = (\psi_i, \omega_i)_{i \in I}$ such that any $\omega_i \in \text{Lip}_k$. Moreover ψ_i is C -bounded on ω_i with a constant independent of $i \in I$.*

Proof: The proof for the compact case (so without boundary) is quite short: We have already defined a suitable inverse atlas by using the exponential map and balls of certain fixed radius $r > 0$, which are obviously Lipschitz.

Turning now to the case with boundary, we have required in this case that $\text{M} \subseteq \widehat{\text{M}}$ with $\widehat{\text{M}} \in \mathbb{M}_{\text{cp}}^k(\mathbb{R}^d)$ a compact ESM without boundary. Our primary goal is now to parameterise the area near the boundary of M suitably, because afterwards we can simply fill up with “exponential” parameterisations in the interior. Therefore, we use the intrinsic tubular neighbourhood of the boundary, which we will parameterise by using an exponential parameterisation of the boundary and extending this. So let $\Gamma = \partial \text{M} \in \mathbb{M}_{\text{cp}}^{k-1}(\mathbb{R}^d)$ be a hypersurface of some $\widehat{\text{M}} \in \mathbb{M}_{\text{cp}}^k(\mathbb{R}^d)$. By conception, we know that Γ is a compact ESM without boundary, whereby there

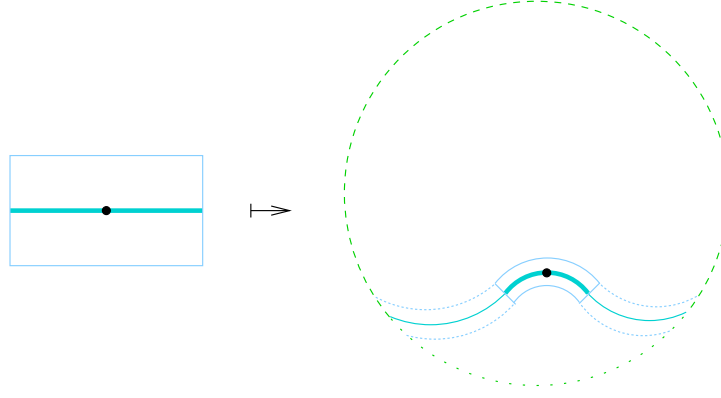


Figure 9.2: Depicted is the step from one parameter space for the intrinsic tubular neighbourhood to the respective part of the intrinsic tubular neighbourhood. The boundary is depicted in teal, the dashed green curve implies M , the dotted green curve completes M to become \widehat{M} . Intrinsic tubular neighbourhood in blue.

is an exponential inverse atlas $\mathbb{A}_\Gamma = \{(\widehat{\psi}_i, \widehat{\omega}_i)\}_{i \in I}$ with finite index set I such that any $\widehat{\psi}_i$ is C -bounded and any $\widehat{\omega}_i$ is a ball of radius $r_\Gamma > 0$. We will now make a parameterisation of the intrinsic tubular neighbourhood out of this. We choose therefore

$$\widehat{\psi}_i : \widehat{\omega}_i \times]-\frac{\delta}{2}, \frac{\delta}{2}[\rightarrow \widehat{M} \quad \widehat{\psi}_i(x, t) = \exp_{\widehat{\psi}_i(x), \widehat{M}}(t \cdot \nu(\widehat{\psi}_i(x))).$$

This yields a C -bounded parameterisation of $U_{\delta/2}^{\widehat{M}}(\Gamma)$ if applied on any $\widehat{\omega}_i$ and $\widehat{\psi}_i$. Moreover, we can demand that the radius r_Γ is the $\delta > 0$ of the intrinsic tubular neighbourhood theorem without harm, as we just have to shrink one or the other sufficiently. The resulting sets $\widehat{\omega}_i \times]-\delta/2, \delta/2[$ are obviously hypercylinders and thus clearly Lipschitz domains.

We will achieve a parameterisation of $U_{\delta/2}^{\widehat{M}}(\Gamma) \cap M$ now by simply restricting the parameter space to $\widehat{\omega}_i \times]0, \delta/2[$ or $\widehat{\omega}_i \times]-\delta/2, 0[$, depending on which side of Γ the desired set M was. This choice shall be named $\widehat{\omega}_i$. Then we have to enhance the resulting inverse atlas $\{(\widehat{\psi}_i, \widehat{\omega}_i)\}_{i \in I}$ parameterizing $U_{\delta/2}^{\widehat{M}}(\Gamma) \cap M$ by sufficiently many pairs $(\exp_{\xi, M}, B_r^k(0))$ for suitable $\xi \in M$ with $d_M(\xi, \Gamma) > \delta/2$ to obtain an inverse atlas for the whole of M , which is no problem by the relative compactness of M in the compact ESM \widehat{M} . \square

9.7 Remark: (1) We can thereby choose a restrictable Lipschitz inverse atlas for an ESM \widehat{M} , which we use in defining Sobolev spaces: We just have to change the last step in the proof of the theorem, where we do not take the upper or lower half of $\widehat{\omega}_i \times]-\delta/2, \delta/2[$, but the whole set, and fill up again by exponentials as parameterisations and balls as parameter spaces, but this time covering all of \widehat{M} .

(2) The construction of suitable smooth maps $T^i : \omega_i \rightarrow TM$ and $N^i : \omega_i \rightarrow NM$ that assign each element of ω_i and thereby also each element of $\psi_i(\omega_i)$ to an orthonor-

mal frame of the respective tangent and normal space is again easily achieved: For T^i we just have to apply orthonormalisation to the Jacobian of the parameterisation ψ_i , and thereby we can also construct N^i after possibly shrinking the parameter spaces suitably.

(3) By this construction it is particularly obvious that in the case without boundary we can always choose the radius of the parameter space balls slightly larger or smaller if needed and still obtain an inverse atlas.

9.2 A Theory of Function Spaces on Embedded Submanifolds

We now present a more detailed, though still brief, revision of important facts for function spaces on ESMs. In particular, we give proofs for the respective results from the main part that were omitted there.

9.2.1 Norm Equivalences for Integer Order Spaces

We begin this section with the proof of Theorem 2.26, which comes along with a useful lemma that states the invariance of integer Sobolev spaces under diffeomorphisms:

9.8 Lemma *If $\Omega \in \mathbb{Lip}_d$ and $\varphi : \Omega \rightarrow \varphi(\Omega)$ is a bidirectionally C-bounded diffeomorphism, then $\|f\|_{W_p^m(\varphi(\Omega))}$ is equivalent to the following norm:*

$$\|f\|_{W_p^m(\Omega, \varphi)} := \|f \circ \varphi\|_{W_p^m(\Omega)}.$$

Proof: The claimed equivalence is actually well known and fairly obvious, but we shall nonetheless give a short proof here to emphasise some aspects of uniformity of constants. We define $z = \varphi(x)$ and obtain for any smooth function f that it holds

$$\|f\|_{W_p^m(\varphi(\Omega))}^p = \sum_{|\alpha| \leq m} \int_{\varphi(\Omega)} |\partial^\alpha f|^p = \sum_{|\alpha| \leq m} \int_{\Omega} |(\partial^\alpha f) \circ \varphi|^p \cdot |\det D\varphi|.$$

Fà di Bruno's formula gives us a tool to bound the partial derivatives of $f_\varphi := f \circ \varphi$ by partials of f (cf. [82, 4.2.1, esp. Thm. 6]): We obtain that any partial derivative of multi-index-order η of f_φ is a linear combination of partials of f to multi-indices β up to order $|\eta|$, and the coefficients are polynomials $P_{\eta, \beta}(\varphi)$ in partial derivatives of φ up to order $|\eta|$, which are known to be globally bounded up to any finite order by C-boundedness:

$$\partial^n f_\varphi = \sum_{1 \leq |\beta| \leq |\eta|} ((\partial^\beta f) \circ \varphi) \cdot P_{\eta, \beta}(\varphi) \implies |\partial^n f_\varphi| \leq c \sum_{1 \leq |\beta| \leq |\eta|} |(\partial^\beta f) \circ \varphi|.$$

Consequently, we can apply Hölder's inequality to obtain

$$|\partial^\alpha f_\varphi|^p \leq c \sum_{|\beta| \leq m} |(\partial^\beta f) \circ \varphi|^p,$$

for some constant c independent of f and φ . Additionally $0 < \varepsilon \leq |\det D\varphi|$ for some fixed ε by C -boundedness and diffeomorphy, so we can deduce that

$$|\partial^\alpha f_\varphi|^p \leq c \sum_{|\beta| \leq m} |(\partial^\beta f) \circ \varphi|^p |\det D\varphi| \leq c \sum_{|\beta| \leq m} |(\partial^\beta f) \circ \varphi|^p.$$

Integration and summation over α yields one of the desired inequalities for smooth functions, and the overall result comes by density. To obtain the other, we just have to reapply this process in the inverse direction, so with φ^{-1} and $1/\det D\varphi$. \square

Proof of Theorem 2.26: Since we have a finite bounded Lipschitz inverse atlas on M and $U_h(M)$, we can restrict ourselves to one pair (ψ, ω) , corresponding $(\Psi, \omega \times B_h^K(0))$ and corresponding $U_{\omega, h} = \Psi(\omega \times B_h^K(0))$. Then, the first inequality is effectively just the statement of Lemma 9.8:

$$a_1 \|F\|_{W_p^m(U_{\omega, h})} \leq \|F \circ \Psi\|_{W_p^m(\omega \times B_h^K)} \leq a_2 \|F\|_{W_p^m(U_{\omega, h})}.$$

Since the overlap count of the sets $\Psi_i(\omega \times B_h^K(0))$ is bounded by definition, we obtain the desired relation by summation. We have to take some care on the uniformity of constants w.r.t. h however. But by taking a close look at the proof of the preceding Lemma 9.8, we see that the extent of the regions never played a role there as long as C -boundedness was guaranteed for a global constant over the regions — which can be required as the regions just get smaller and are suitably nested. So we can directly conclude the desired inequality by summing over all charts, as we know that any Ψ is bidirectionally C -bounded with a global constant valid for all parameterisations.

Turning to the second relation, we just have to achieve that for any (ψ, ω) with corresponding $(\Psi, \omega \times B_h^K(0))$ and $\vec{F}_\psi := (E_N f) \circ \Psi$ we have the inequality

$$b_1 h^{\kappa/p} \|f\|_{W_p^m(\psi(\omega))} \leq \|\vec{F}_\psi\|_{W_p^m(\omega \times B_h^K)} \leq b_2 h^{\kappa/p} \|f\|_{W_p^m(\psi(\omega))}.$$

This is sufficient because the overall result can then be deduced by finite summation. So it actually suffices to provide

$$b_1 h^{\kappa/p} \|f\|_{W_p^m(\psi(\omega))} \leq \|\vec{F}_\psi\|_{W_p^m(\omega \times B_h^K)} \quad \text{and} \quad \|\vec{F}_\psi\|_{W_p^m(\omega \times B_h^K)} \leq b_2 h^{\kappa/p} \|f\|_{W_p^m(\psi(\omega))}.$$

This is easy to see: By definition we have $\vec{F}_\psi(x, y) = f(\psi(x))$ for $x \in \omega$ and $y \in B_h^\kappa$. Consequently, any $\partial^\alpha \vec{F}_\psi(x, z)$ will vanish if at least one of the last κ entries of α is nonzero. And if all of these last κ entries in α are zero, then $\partial^\alpha \vec{F}_\psi(x, z)$ coincides with the corresponding $\partial^\alpha (f \circ \psi)(x)$ and is thus constant in z . So for any $x \in \omega$

$$\int_{B_h^\kappa} \sum_{|\alpha| \leq m} |\partial^\alpha \vec{F}_\psi(x, z)|^p = c \cdot h^\kappa \sum_{|\alpha| \leq m} |\partial^\alpha (f \circ \psi)(x)|^p,$$

which gives the desired result by Fubini and insertion. \square

9.2.2 Embeddings in Sobolev Spaces

The following proposition sums up a number of relevant embedding properties of Sobolev spaces into one another and into spaces of continuous functions that we refer to every once in a while and that are stated here for the readers convenience (cf. [1, Th. 5.4], [2, Th. 6.3]):

9.9 Proposition — Integer Sobolev Embedding —

Let $\Omega \in \mathbb{Lip}_d^*$, $m, \mu \in \mathbb{N}_0$ and $p, q \in [1, \infty[$. Then we have the continuous embeddings

1. $W_p^m(\Omega) \hookrightarrow W_p^\mu(\Omega)$, if $\mu \leq m$.
2. $W_p^m(\Omega) \hookrightarrow C(\Omega)$ if $m > \frac{d}{p}$ and $p > 1$.

9.10 Proposition — Rellich-Kondrachov Embedding —

The embedding $W_p^m(\Omega) \hookrightarrow W_p^\mu(\Omega)$ from the last proposition is compact if $\mu < m$. That means, for any bounded sequence in $W_p^m(\Omega)$ there is a subsequence that is convergent as a sequence of $W_p^\mu(\Omega)$.

All of the above embedding results also hold for ESMs. To see this, note that $f \in W_p^m(M)$ precisely if and only if for any (ψ_i, ω_i) in the finite inverse atlas with each ψ_i being C -bounded up to order m it holds for any $i \in I$ that $f \circ \psi_i \in W_p^m(\omega_i)$. On each ω_i we can apply the respective embedding, and since the inverse atlas is finite, we can simply use the maximal necessary constant over all parameterisations.

Only the Rellich-Kondrachov embedding requires some further simple arguments: If $(g_n)_{n \in \mathbb{N}}$ is bounded in $W_p^m(M)$, then the function $g_n \circ \psi$ is bounded in $W_p^m(\omega)$ for any $n \in \mathbb{N}$ and any (ψ, ω) in the inverse atlas. So in particular there is a subsequence $(g_n^1)_{n \in \mathbb{N}}$ of $(g_n)_{n \in \mathbb{N}}$ such that $(g_n^1 \circ \psi_1)_{n \in \mathbb{N}}$ is convergent in $W_p^\mu(\omega_1)$. We repeat this argument for $(g_n^1)_{n \in \mathbb{N}}$ as an obviously bounded set over (ψ_2, ω_2) to obtain a subsequence $(g_n^2)_{n \in \mathbb{N}}$ of $(g_n^1)_{n \in \mathbb{N}}$ that is convergent in $W_p^\mu(\omega_2)$. By repeating this process until all pairs of the finite inverse atlas are covered we obtain the desired Rellich-Kondrachov Theorem.

We also have an embedding theorem that corresponds to Proposition 9.9 in the fractional case⁽¹⁾:

9.11 Proposition — Fractional Sobolev Embedding —

Let $\Omega \in \mathbb{Lip}_d$, $0 \leq \sigma \leq s < 1$ and $\mu, m \in \mathbb{N}_0$. Then the following embeddings hold:

1. $H^{m+s}(\Omega) \hookrightarrow H^{\mu+\sigma}(\Omega)$ if $\mu + \sigma \leq m + s$.
2. $H^{m+s}(\Omega) \hookrightarrow C(\Omega)$ if $m + s > \frac{d}{2}$.

All relations also hold for $\Omega = \mathbb{R}^d$.

9.2.3 A Note on Besov Spaces

Among many different choices to define these very general class of function spaces, we follow the concept applied in [68] and presented e.g. in [100, 1.11.9]. As already stated elsewhere and presented e.g. in [77, 96, 97, 98, 99, 100], particularly [96, Sect. 2.3.2, Sect 2.7.1], [98, Sect. 2.3, 2.8, 4.2, 4.6], [99, Sect. 2, Th. 2.13], our Slobodeckij Hilbert spaces appear as special cases of these Besov spaces. Moreover, these Besov spaces can be obtained by a concept called *function space interpolation* (cf. [14, 77, 96, 97, 98, 100]), and as the Slobodeckij spaces appear as special Besov spaces, we can employ the powerful results of that concept in our setting. We shall not go into detail here and refer the interested reader to the profound amount of literature treating this topic. We just give the definition and a simple but important example:

9.12 Definition For real $r = m + s$ with $m \in \mathbb{N}_0$, $0 \leq s < 1$ and $1 \leq p, q < \infty$, we define the *Besov space* $B_{p,q}^r(\mathbb{R}^d)$ as the space of functions in $W_p^m(\mathbb{R}^d)$ for which

$$\int_{\mathbb{R}} \frac{1}{t} (t^{-r} \omega_{m+1}(f, t)_p)^q dt < \infty.$$

Therein, $\omega_m(f, t)_p$ is the m th modulus of smoothness of f w.r.t. t , so for the difference operator $\Delta_\nu(f) := f(\cdot + \nu) - f(\cdot)$ it is given as

$$\omega_m(f, t)_p = \sup_{\|\nu\|_2 \leq t} \|\Delta_\nu^m(f)\|_{L_p(\mathbb{R}^d)}.$$

9.13 Example: Any univariate, compactly supported function that is piecewise constant with a finite set of breaks is in the Besov space $B_{p,p}^\varepsilon(\mathbb{R}^d)$ for any $0 < \varepsilon < 1/p$. This can be seen as follows: We restrict ourselves to the case of a function f that is 1 in some $[0, t_0]$ and vanishes elsewhere. Then we can bound

⁽¹⁾Cf. [1, 7.57ff],[2, 7.30ff,7.57ff],[32] [80], [96, Sect. 2.3.2, Sect 2.7.1], [100, Sect. 1.11, 4.1] and the identification from [2, p. 255]

$$\sup_{|\nu| \leq t} \|\Delta_\nu^1(f)\|_{L_p(\mathbb{R})} \leq \left(\int_{-\min(t, t_0)}^0 1 \, dt + \int_{t_0 - \min(t, t_0)}^{t_0} 1 \, dt \right)^{1/p} \leq c \min(t, t_0)^{1/p}.$$

Inserting this gives finiteness of the respective seminorm precisely if $s < \frac{1}{p}$. As for the modulus of smoothness it holds due to [89, Thm. 2.29]

$$\omega_{m+1}(f, t)_p \leq t^m \omega_1(D^m f, t)_p,$$

we can thus derive in particular that any univariate B-spline of order m with overall knot multiplicity one is in $B_{p,p}^r(\mathbb{R}^d)$ for any $r < m - 1 + \frac{1}{p}$.

9.2.4 Consequences of Sobolev Space Interpolation

We will also make use of the *interpolation property* (cf. [77, Th. 1.1.6], [89, Th. 6.30], [14, Def. 2.4.1], [96, Sect. 2.4.1]):

9.14 Proposition *Let $\Omega_1 \in \text{Lip}_{d_1}^*$, $\Omega_2 \in \text{Lip}_{d_2}^*$. Let $r = \theta r_1 + (1-\theta)r_2$ for $\theta \in]0, 1[$ and reals $0 \leq r_1 \leq r_2 < \infty$ and let $\varrho = \theta \varrho_1 + (1-\theta)\varrho_2$ for reals $0 \leq \varrho_1 \leq \varrho_2 < \infty$. If $\Lambda : H^{r_i}(\Omega_1) \mapsto H^{\varrho_i}(\Omega_2)$ is bounded for $i = 1, 2$, then $\Lambda : H^r(\Omega_1) \mapsto H^\varrho(\Omega_2)$ is bounded as well and*

$$\|\Lambda\|_{H^r \rightarrow H^\varrho} \leq c_\Omega \|\Lambda\|_{H^{r_1} \rightarrow H^{\varrho_1}}^\theta \|\Lambda\|_{H^{r_2} \rightarrow H^{\varrho_2}}^{(1-\theta)}.$$

If a family $\{\Lambda_h\}_{0 < h < h_0}$ of such operators satisfies

$$\|\Lambda_h\|_{H^{r_1} \rightarrow H^{\varrho_1}}^\theta \leq c_1 h^{\lambda_1} \quad \text{and} \quad \|\Lambda_h\|_{H^{r_2} \rightarrow H^{\varrho_2}}^{(1-\theta)} \leq c_2 h^{\lambda_2},$$

then we have in particular the relation $\|\Lambda_h\|_{H^r \rightarrow H^\varrho} \leq c h^{\lambda_1 \cdot \theta + \lambda_2 \cdot (1-\theta)}$.

Proof: The result for $\Omega_j = \mathbb{R}^{d_j}$ is a consequence of [77, Th. 1.1.6] and the fact that our Slobodeckij spaces are such interpolation spaces for interpolation of Hilbert spaces. The latter is a consequence of the fact that the interpolation methods that are employed in obtaining them have the respective property, cf. the theorems 3.1.2, 3.2.2 and 4.1.4 in [14]. In particular, the choice $r_2 = r_1$ or $\varrho_2 = \varrho_1$ is valid by [14, Th. 6.4.5].

The respective result for $\Omega_j \in \text{Lip}_{d_j}$ comes by application of the universal extension operator: We apply the operator $E_2 \Lambda R_1$ for universal extensions $E_j : H(\Omega_j) \rightarrow H(\mathbb{R}^{d_j})$ and restrictions $R_j : H(\mathbb{R}^{d_j}) \rightarrow H(\Omega_j)$, which is clearly bounded as a map from $H^{r_i}(\mathbb{R}^{d_1})$ to $H^{\varrho_i}(\mathbb{R}^{d_2})$. By the interpolation property, it is then also bounded as a map from $H^r(\mathbb{R}^{d_1})$ to $H^\varrho(\mathbb{R}^{d_2})$ and

$$\|E_2 \Lambda R_1\|_{H^r \rightarrow H^\varrho} \leq c \|E_2 \Lambda R_1\|_{H^{r_1} \rightarrow H^{\varrho_1}}^\theta \|E_2 \Lambda R_1\|_{H^{r_2} \rightarrow H^{\varrho_2}}^{(1-\theta)} \leq c \|\Lambda\|_{H^{r_1} \rightarrow H^{\varrho_1}}^\theta \|\Lambda\|_{H^{r_2} \rightarrow H^{\varrho_2}}^{(1-\theta)}.$$

Consequently, we obtain for any $f \in H^r(\Omega_1)$

$$\begin{aligned}
\|\Lambda f\|_{H^\theta(\Omega_2)} &\leq c_2 \|E_2 \Lambda R_1 E_1 f\|_{H^\theta(\mathbb{R}^{d_2})} \\
&\leq c \|E_2 \Lambda R_1\|_{H^r \rightarrow H^\theta} \|E_1 f\|_{H^r(\mathbb{R}^{d_1})} \\
&\leq c \|\Lambda\|_{H^{r_1} \rightarrow H^{\theta_1}}^\theta \|\Lambda\|_{H^{r_2} \rightarrow H^{\theta_2}}^{(1-\theta)} \|E_1 f\|_{H^r(\mathbb{R}^{d_1})} \\
&\leq c \|\Lambda\|_{H^{r_1} \rightarrow H^{\theta_1}}^\theta \|\Lambda\|_{H^{r_2} \rightarrow H^{\theta_2}}^{(1-\theta)} \|f\|_{H^r(\Omega_1)}.
\end{aligned}$$

The additional conclusion is now obvious by insertion of the respective operator norms. \square

An important consequence of the function space interpolation theory is that also fractional spaces are invariant under diffeomorphisms. From this we can deduce that they remain also unaffected if we consider the tubular neighbourhood of an ESM on the one hand directly and on the other hand by a finite set of parameterisations subordinate to a foliation. We shall achieve the latter by a number of intermediate steps:

9.15 Lemma *If $\Omega \in \mathbb{Lip}_d$ and $\varphi : \Omega \rightarrow \varphi(\Omega)$ is a bidirectionally C -bounded diffeomorphism, then $\|f\|_{H^{m+s}(\varphi(\Omega))}$ is equivalent to the following norm:*

$$\|f\|_{H^{m+s}(\Omega, \varphi)} := \|f \circ \varphi\|_{H^{m+s}(\Omega)}.$$

Proof: To see this, we construct the operator $\Lambda_\varphi : H^{m_i}(\varphi(\Omega)) \rightarrow H^{m_i}(\Omega)$ by $f \mapsto f \circ \varphi$ for $i = 1, 2$ and suitable m_i such that for an appropriate choice of θ it holds $m+s = \theta m_1 + (1-\theta)m_2$. By Lemma 9.8 and the interpolation property, this operator is also bounded as an operator $\Lambda_\varphi : H^{m+s}(\varphi(\Omega)) \rightarrow H^{m+s}(\Omega)$. This gives one of the required inequalities. The other follows by application of the same concept to the inverse diffeomorphism and the map

$$\Lambda_{\varphi^{-1}} : H^{m_i}(\Omega) \rightarrow H^{m_i}(\varphi(\Omega)), \quad g \mapsto g \circ \varphi^{-1},$$

which gives the desired result for the choice $g = f \circ \varphi$. \square

9.16 Lemma *Let $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ and let $U(M) = U_\rho(M)$ be a fixed tubular neighbourhood of M . Let $\mathbb{U} = (\Psi_i, \Omega_i)_{i=1}^n$ be an inverse atlas of $U(M)$ subordinate to the normal foliation. Then there is an open cover $\{\Theta_j\}_{j=1}^{n+1}$ of \mathbb{R}^d such that*

1. Θ_j is bounded for any $j = 1, \dots, n$
2. $\Theta_{n+1} \cap \Psi_i(\Omega_i) = \emptyset$ for all $i = 1, \dots, n$
3. $\Theta_j \cap U(M) = \Psi_j(\Omega_j)$

and a smooth partition of unity $\{\chi_i : \mathbb{R}^d \rightarrow [0, 1]\}_{i=1}^n$ subordinate to this open cover.

Proof: We first give the proof for an ESM without boundary: We can find some $\varrho^* > \varrho$ such that $U_{\varrho^*}(\mathbb{M})$ still has the closest point property and can be parameterised by a suitable modification of the inverse atlas for $U_{\varrho^*}(\mathbb{M})$. To accomplish this, we just have to extend a little further in normal directions. This modified inverse atlas for $U_{\varrho^*}(\mathbb{M})$ shall be denoted $\mathbb{U}^* = (\Psi_i^*, \Omega_i^*)_{i=1}^n$. We choose $\Theta_i = \Psi_i^*(\Omega_i^*)$ for $i = 1, \dots, n$. Moreover, the closure of

$$U(\mathbb{M}) = \bigcup_{i=1}^n \Psi_i(\Omega_i)$$

is a compact set, and thus its complement is open and we choose it as Θ_{n+1} . This already completes the construction for the case without boundary. In case \mathbb{M} has a boundary, then we also know that $\mathbb{M} \subseteq \widehat{\mathbb{M}}$ without boundary, and we can choose an inverse atlas $\mathbb{A}_{\mathbb{M}} \in \mathbb{I}(\mathbb{M})$ for \mathbb{M} with a corresponding restrictable inverse atlas $\mathbb{A}_{\widehat{\mathbb{M}}} \in \mathbb{I}_R(\mathbb{M})$ of $\widehat{\mathbb{M}}$, for example according to Theorem 9.6 and Corollary 9.7. Then we construct the open cover $\{\Theta_j^+\}$ for $\widehat{\mathbb{M}}$ first. Afterwards, we skip the unbounded set and any Θ_j^+ that was constructed for a pair (Ψ^+, Ω^+) that does not correspond to some (Ψ, Ω) and (ψ, ω) of the inverse atlas for \mathbb{M} . Then we choose again the additional unbounded set Θ_{n+1} as the complement of the closure of

$$\bigcup_{i=1}^n \Psi_i(\Omega_i).$$

Finally, the existence of a smooth partition of unity is due to [73, Thm. 2.25]. \square

The most important feature of this open cover is that whenever there is a function $F : U(\mathbb{M}) \rightarrow \mathbb{R}$ and a set of functions $F_i : \Psi_i(\Omega_i) \rightarrow \mathbb{R}$ such that $F_i = F|_{\Psi_i(\Omega_i)}$, then F and the function

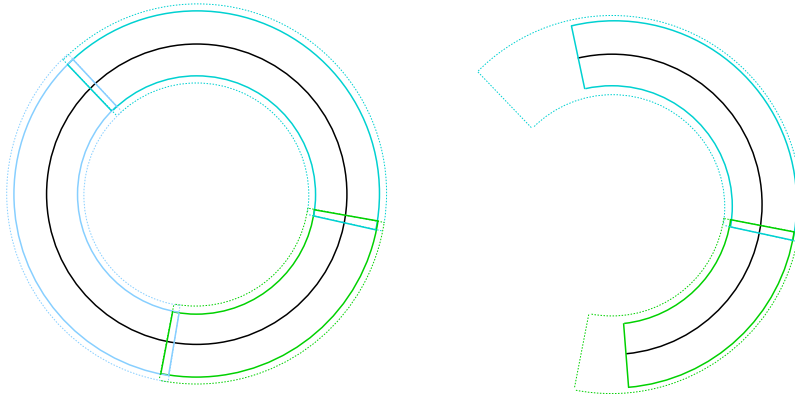


Figure 9.3: Depicted is on the left a circle with three corresponding extended cover sets in solid green, teal and blue and their corresponding Θ_i in dotted green, teal and blue. Depicted on the right is what remains for a subarc of the circle as an ESM with boundary. Note in particular that the cover elements do not change

$$\sum_{i=1}^n \chi_i \cdot F_i$$

coincide on $U(M)$. This can be deduced from the fact that $\Theta_j \cap \bigcup_{i=1}^n \Psi_i(\Omega_i) = \Psi_j(\Omega_j)$ for any $j = 1, \dots, n$ and that the sets $\Psi_i(\Omega_i)$ cover $U(M)$ themselves. We will make use of this property now and in the further course of this section:

9.17 Theorem *Let $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ and let $U(M) = U_\varrho(M)$ be a fixed tubular neighbourhood of M . Let $\mathbb{U}_M = (\Psi_i, \Omega_i)_{i \in I}$ be an inverse atlas of $U(M)$ subordinate to the normal foliation. Then there are fixed $a_1, a_2 > 0$ such that for any $F \in H^r(U(M))$*

$$a_1 \|F\|_{H^r(U(M))} \leq \sum_{i \in I} \|F \circ \Psi_i\|_{H^r(\Omega_i)} \leq a_2 \|F\|_{H^r(U(M))}.$$

Moreover, for any $f \in H^r(M)$ and suitable $b > 0$ it holds

$$\|E_N f\|_{H^r(U(M))} \leq b \|f\|_{H^r(M)}.$$

Proof: With the last lemmas, it is clear that it holds for any $i \in I = \{1, \dots, |I|\}$

$$\sum_{i \in I} \|F \circ \Psi_i\|_{H^r(\Omega_i)} \leq c \sum_{i \in I} \|F\|_{H^r(\Psi_i(\Omega_i))} \leq a_2 \|F\|_{H^r(U(M))}.$$

It is also clear by the same result that conversely

$$\|F\|_{H^r(\Psi_i(\Omega_i))} \leq c \|F \circ \Psi_i\|_{H^r(\Omega_i)}.$$

But the step from the sum over the $\|F\|_{H^r(\Psi_i(\Omega_i))}$ to $\|F\|_{H^r(U(M))}$ is subtle, because it does not come directly by the definition. To prove this, we have to consider the universal continuous extension operators $E_i : H^r(\Psi_i(\Omega_i)) \rightarrow H^r(\mathbb{R}^d)$ for each pair (Ψ_i, Ω_i) . For given F , they give us functions $F_i \in H^r(\mathbb{R}^d)$ that coincide with F in $\Psi_i(\Omega_i)$ and satisfy $\|F_i\|_{H^r(\mathbb{R}^d)} \leq c_i \|F\|_{H^r(\Psi_i(\Omega_i))}$. Now we take the previously constructed open cover and partition of unity and achieve by the triangle and Hölder inequality the missing step via

$$\|F\|_{H^r(U(M))} = \left\| \sum \chi_i F_i \right\|_{H^r(U(M))} \leq \left\| \sum \chi_i F_i \right\|_{H^r(\mathbb{R}^d)} \leq c \sum_{i \in I} \|F_i\|_{H^r(\mathbb{R}^d)} \leq c \sum_{i \in I} \|F\|_{H^r(\Psi_i(\Omega_i))}.$$

To draw the conclusion on the normal extension, it suffices to prove the respective equivalence on $H^r(\omega_i)$ and $H^r(\Omega_i)$ for arbitrary $i \in I$. This can be achieved by applying the interpolation property again: We have seen in 2.26 that for fixed h (which is the case now) the operator $E_N : H^{m_j}(\omega_i) \rightarrow H^{m_j}(\Omega_i)$ is bounded for $j = 1, 2$ and suitable m_j such that for an appropriate choice of θ it holds $r = \theta m_1 + (1 -$

$\theta)m_2$. Consequently, it is also continuous as a map from $H^r(\omega_i)$ to $H^r(\Omega_i)$, which is precisely the desired relation. \square

9.2.5 Trace Theorems

We will now revise the trace theorems and provide proofs and / or literature references as necessary:

9.18 Theorem — Integer Trace Theorem —

1. Let $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ be equipped with finite inverse atlas $\mathbb{A}_M = \{(\psi_i, \omega_i)\}_{i \in I} \in \mathbb{II}(M)$ and let $U(M) \in \text{Lip}_d$ be some ambient tubular neighbourhood of M with fixed extent $\varrho > 0$. Let $F \in W_p^m(U(M))$ for some $1 \leq p < \infty$ and $m \in \mathbb{N}$. Then $T_M F \in W_p^\mu(M)$ for any $\mu \in \mathbb{N}_0$ with $\mu < m - \frac{d-k}{p}$ ($\mu \leq m - \frac{d-k}{p}$ in case $p = 1$) and

$$\|T_M F\|_{W_p^\mu(M)} \leq c \|F\|_{W_p^m(U(M))}.$$

2. Let $f \in W_p^m(M)$ for some $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ and some $1 \leq p < \infty$ and $m \in \mathbb{N}$. Take some open and bounded $M_0 \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ with $M_0 \subseteq M$ that has nonempty smooth boundary Γ . Then $T_\Gamma f \in W_p^\mu(\Gamma)$ for any $\mu < m$ and

$$\|T_\Gamma f\|_{W_p^\mu(\Gamma)} \leq c \|f\|_{W_p^m(M_0)}.$$

Proof: The first relation is known to be true if $U(M)$ is an open domain Ω in \mathbb{R}^d and $M \in \text{Lip}_k$ is given as $\Omega \cap \mathbb{R}^k$ due to [1, Th. 5.4]. The corresponding claim for ESMs is then a direct consequence of this fact if we consider Lemma 9.8, where we gave equivalence of norms under C -bounded diffeomorphisms.

The second claim ultimately is again a consequence of the first: We choose first an arbitrary (ψ, ω) according to the inverse atlas of M . Then clearly $\omega_\Gamma := \psi^{-1}(\Gamma \cap \psi(\omega))$ is just a subset of \mathbb{R}^{k-1} if we take a suitable restrictable inverse atlas, for example the one we presented in the construction process of the first section of this appendix. Then we can apply the first statement to $f \circ \psi$ on ω with respect to ω_Γ and are already done. \square

9.19 Theorem — Fractional Trace Theorem —

Let $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ have finite inverse atlas $\mathbb{A}_M = \{(\psi_i, \omega_i)\}_{i \in I} \in \mathbb{II}(M)$ and let $U(M) \in \text{Lip}_d$ be some tubular neighbourhood of M with fixed extent $\varrho > 0$ and extended inverse atlas $\{(\Psi_i, \Omega_i)\}_{i \in I} \in \mathbb{II}_N^{\text{ex}}(M)$ subordinate to \mathbb{A}_M . Let $F \in H^r(U(M))$ for $r > \frac{d-k}{2}$. Then $T_M F \in H^\varrho(M)$ for $\varrho = r - \frac{d-k}{2} > 0$ and

$$\|T_M F\|_{H^\varrho(M)} \leq c \|F\|_{H^r(U(M))}.$$

If conversely $g \in H^\varrho(\mathbb{M})$ then there is a bounded extension operator $E_M^U : H^\varrho(\mathbb{M}) \rightarrow H^r(U(\mathbb{M}))$, so

$$\|E_M^U g\|_{H^r(U(\mathbb{M}))} \leq c \|g\|_{H^\varrho(\mathbb{M})}.$$

Again, this extension operator is independent of ϱ and thus universally applicable for any $\varrho > 0$ and $r = \varrho + \kappa/2$. All statements remain valid if one replaces $U(\mathbb{M})$ by \mathbb{M} and \mathbb{M} by some ESM $\Gamma \in \mathbb{M}_{\text{bd}}^\ell(\mathbb{M})$ for $0 < \ell < k$.

Proof: First of all, the respective relation holds for $\mathbb{R}^d, \mathbb{R}^k$ due to [3, Sect. 1.10, 3.3] or [96, 2.7.2]. For the step from $\mathbb{R}^d, \mathbb{R}^k$ to some set $\Omega \in \text{Lip}_d$ and $\Omega^k = \Omega \cap \mathbb{R}^k$ we rely on our universal extensions as stated in Proposition 2.29, particularly the extension $E_\Omega^{\mathbb{R}^d}$. Thereby we obtain

$$\|T_{\Omega^k} F\|_{H^\varrho(\Omega^k)} \leq \|T_{\mathbb{R}^k} E_\Omega^{\mathbb{R}^d} F\|_{H^\varrho(\mathbb{R}^k)} \leq c \|E_\Omega^{\mathbb{R}^d} F\|_{H^r(\mathbb{R}^d)} \leq c \|F\|_{H^r(\Omega)}.$$

Similarly, we get for the bounded extension $E_{\Omega^k}^\Omega := R_\Omega E_{\mathbb{R}^k}^{\mathbb{R}^d} E_{\Omega^k}^{\mathbb{R}^k}$ that

$$\|E_{\Omega^k}^\Omega g\|_{H^r(\Omega)} \leq \|E_{\mathbb{R}^k}^{\mathbb{R}^d} E_{\Omega^k}^{\mathbb{R}^k} g\|_{H^r(\mathbb{R}^d)} \leq c \|E_{\Omega^k}^{\mathbb{R}^k} g\|_{H^\varrho(\mathbb{R}^k)} \leq c \|g\|_{H^\varrho(\Omega^k)}.$$

The corresponding tracing claims for ESMs and suitable neighbourhoods can now be concluded by application of the respective relations on domains on each element of the inverse atlas and corresponding inverse atlas of the neighbourhood subordinate to the normal foliation. Note therein in particular that due to Lemmas 9.8 and 9.15, the respective norms and spaces are equivalent under diffeomorphic transformations. For the extension part we have to work a bit harder: Clearly, we can construct suitable extensions from each ω_i into corresponding Ω_i . Consequently, we can also extend from $\psi_i(\omega_i)$ to $\Psi_i(\Omega_i)$ by norm equivalences of Lemmas 9.8 and 9.15, and even from there into all of \mathbb{R}^d . So we obtain some functions $G_i \in H^r(\mathbb{R}^d)$ such that

$$\|G_i\|_{H^r(\mathbb{R}^d)} \leq c_i \|g \circ \psi_i\|_{H^\varrho(\omega_i)} \quad \forall i \in I,$$

and consequently

$$\sum_{i \in I} \|G_i\|_{H^r(\mathbb{R}^d)} \leq \sum_{i \in I} c_i \|g \circ \psi_i\|_{H^\varrho(\omega_i)} \leq c \|g\|_{H^\varrho(\mathbb{M})}.$$

But these G_i do not necessarily coincide as one overall extension. Instead, we will have to blend the resulting extensions to obtain such. Therefore, we take again the open cover and partition of unity from Lemma 9.16. Then an application of Hölder's inequality to the newly defined

$$G := \sum_{i \in I} G_i \cdot \chi_i$$

shows that because any χ_i has compact support the blended function G satisfies

$$\|G\|_{H^r(\mathbb{R}^d)} \leq c \sum_{i \in I} \|G_i\|_{H^r(\mathbb{R}^d)} \leq c \|g\|_{H^p(M)}.$$

By construction, the trace of G on M coincides with g . Moreover, since both the extension operators from the domains ω_i into \mathbb{R}^k and from \mathbb{R}^k into \mathbb{R}^d and the restriction of these to Ω_i are independent of ρ , so is our overall operator.

For the respective relation in case of submanifolds of an ESM, we can rely on the restrictable inverse atlas. Then the desired relations can be deduced easily in the same way. In particular for the extension from Γ to M , we can just apply the extension from Γ to some \mathbb{R}^d and take its trace on M . \square

If we reconsider this proof, the following corollary is a particular conclusion:

9.20 Corollary — Chart Trace Theorem —

In the setting of the last theorem it holds for any pair (ψ, ω) from the inverse atlas $\mathbb{A}_M \in \mathbb{II}(M)$, corresponding $(\Psi, \Omega) \in \mathbb{U}_M \in \mathbb{II}_N^{\text{ex}}(M)$ and $F \in H^r(U(M))$ that

$$\|T_\omega(F \circ \Psi)\|_{H^p(\omega)} \leq c \|F\|_{H^r(\Psi(\Omega))} \leq c \|F\|_{H^r(U(M))}.$$

Conversely, there is a bounded extension operator $E_\omega^U : H^p(\omega) \rightarrow H^r(U(M))$ such that for any g with $g \circ \psi \in H^p(\omega)$

$$\|E_\omega^U g\|_{H^r(U(M))} \leq c \|(g \circ \psi)\|_{H^p(\omega)}.$$

We also give a proof that taking the trace of foliation based extensions represents an identity operation:

9.21 Theorem — Foliation Trace Theorem —

Let $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ have the finite inverse atlas $\mathbb{A}_M = \{(\psi_i, \omega_i)\}_{i \in I} \in \mathbb{II}(M)$ and let $U(M) \in \mathbb{Lip}_\rho$ be some tubular neighbourhood of M with fixed extent $\rho > 0$. If then $f \in W_p^m(M)$ it holds $T_M E_N f \in W_p^m(M)$ and

$$\|f - T_M E_N f\|_{W_p^m(M)} = 0.$$

Proof: There is a sequence $(f_n)_{n \in \mathbb{N}}$ of smooth functions approximating f in $W_p^m(M)$. Thereby, $(E_N f_n)_{n \in \mathbb{N}}$ provides a sequence in $W_p^m(U(M))$ that approximates

$E_N f$ in $W_p^m(U(M))$ by Theorem 2.26. As the trace is defined via completion, we have in the $H^m(M)$ -sense

$$T_M E_N f = \lim_{n \rightarrow \infty} T_M E_N f_n = \lim_{n \rightarrow \infty} f_n = f.$$

□

And finally, we also give a proof for the existence of continuous extensions on ESMs:

9.22 Theorem — Manifold Extension Theorem —

Let $M \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ be equipped with inverse atlas $\mathbb{A}_M = \{(\psi_i, \omega_i)\}_{i=1}^n \in \mathbb{I}(M)$. Let further $M_0 \in \mathbb{M}_{\text{bd}}^k(\mathbb{R}^d)$ be an open subdomain $M_0 \Subset M$ that is an ESM of dimension k in its own right and $r > 0$. Then there is an extension operator $E : H^r(M_0) \rightarrow H^r(M)$ such that for any $r > 0$ and any $g \in H^r(M_0)$

$$\|Eg\|_{H^r(M)} \leq c \|g\|_{H^r(M_0)}.$$

This holds also if one replaces M_0 by an arbitrary parameter space ω with corresponding parameterisation ψ according to the inverse atlas in the sense

$$\|E_\omega^M g\|_{H^r(M)} \leq c \|g \circ \psi\|_{H^r(\omega)}.$$

Proof: We obtain a suitable $U(M_0)$ by restriction. Further, by the fractional trace theorem there is an extension $E_{M_0}^{U(M_0)} : H^r(M_0) \rightarrow H^{r+\kappa/2}(U(M_0))$ that is continuous, and there is a continuous extension $E_{U(M_0)}^{\mathbb{R}^d} : H^{r+\kappa/2}(U(M_0)) \rightarrow H^{r+\kappa/2}(\mathbb{R}^d)$ by Proposition 2.29. This gives with the restriction operator $R_{U(M)} : H^{r+\kappa/2}(\mathbb{R}^d) \rightarrow H^{r+\kappa/2}(U(M))$ and $T_M : H^{r+\kappa/2}(U(M)) \rightarrow H^r(M)$ the overall bounded operator

$$E = T_M \cdot R_{U(M)} \cdot E_{U(M_0)}^{\mathbb{R}^d} \cdot E_{M_0}^{U(M_0)},$$

that is continuous by construction. The relation on a single parameter space comes similarly by the chart trace theorem. □

9.2.6 Friedrichs' Inequality

Finally, we will also provide proofs for the two versions of Friedrichs' inequality in the following:

9.23 Theorem — Multicodimensional Friedrichs' Inequality —

Let $\omega \in \text{Lip}_k$ and let $\Omega_h = \omega \times B_h^k[0]$ for $0 < h < h_0$. Let $F \in W_p^k(\Omega_h)$ for some $1 \leq p < \infty$ be a continuous function that vanishes on ω . Then we have the relation

$$\|F\|_{L_p(\Omega_h)}^p \leq c \sum_{\ell=1}^K h^{p \cdot \ell} \sum_{\substack{|\alpha|=\ell \\ \alpha_1=\dots=\alpha_K=0}} \|\partial^\alpha F\|_{L_p(\Omega_h)}^p.$$

Proof: We can demand F to be smooth, as the general relation then follows by completion. We start with an iterated application of the fundamental theorem of calculus:

$$\begin{aligned} F(x, z_1, \dots, z_K) &= \int_0^{z_1} \partial_{k+1} F(x, \zeta_1, z_2, \dots, z_K) d\zeta_1 + F(x, 0, z_2, \dots, z_K) \\ &= \int_0^{z_2} \int_0^{z_1} \partial_{k+2} \partial_{k+1} F(x, \zeta_1, \zeta_2, z_3, \dots, z_K) d\zeta_1 d\zeta_2 + \int_0^{z_2} \partial_{k+2} F(x, 0, \zeta_2, z_3, \dots, z_K) \\ &\quad + \int_0^{z_1} \partial_{k+1} F(x, \zeta_1, 0, z_3, \dots, z_K) + F(x, 0, 0, z_3, \dots, z_K) \\ &= \iiint_{0..0}^{z_1, \dots, z_K} \partial_{k+1, \dots, k+K}^\kappa F(x, \zeta_1, \dots, \zeta_K) d\zeta + \dots + \sum_{i=1}^K \int_0^{z_i} \partial_{i+k} F(x, 0, \dots, 0, \zeta_i, 0, \dots, 0) d\zeta_i \\ &\quad + F(x, 0, \dots, 0). \end{aligned}$$

By assumption $F(x, 0) = 0$, so the last summand vanishes. For any other summand, we can apply Hölder's inequality to the function $1 \cdot g$ for integrand g for the spaces L_p and L_{p^*} with the Hölder-dual $p^* = p/(p-1)$ of p , after using Jensen's inequality $\|\cdot\|_1^p \leq c_1 \|\cdot\|_p^p \leq c_2 \|\cdot\|_1^p$, to obtain that

$$\begin{aligned} |F(x, z_1, \dots, z_K)|^p &\leq c \cdot |z_1 \cdot \dots \cdot z_K|^{\frac{p}{p^*}} \iiint_{0..0}^{z_1, \dots, z_K} |\partial_{k+1, \dots, k+K}^\kappa F(x, \zeta_1, \dots, \zeta_K)|^p d\zeta + \dots \\ &\quad + c \cdot \sum_{i=1}^K |z_i|^{\frac{p}{p^*}} \int_0^{z_i} |\partial_{i+k} F(x, 0, \dots, 0, \zeta_i, 0, \dots, 0)|^p d\zeta_i \\ &\leq c \cdot |z_1 \cdot \dots \cdot z_K|^{\frac{p}{p^*}} \int_{B_h^\kappa[0]} |\partial_{k+1, \dots, k+K}^\kappa F(x, \zeta_1, \dots, \zeta_K)|^p d\zeta + \dots \\ &\quad + c \cdot \sum_{i=1}^K |z_i|^{\frac{p}{p^*}} \int_{-h}^h |\partial_{i+k} F(x, 0, \dots, 0, \zeta_i, 0, \dots, 0)|^p d\zeta_i \end{aligned}$$

We have for $1 \leq j \leq K$, where we consider without restriction the first j variables of the normal part, that by the transformation law

$$\begin{aligned} &\int_{B_h^j[0]} |\partial_{k+1, \dots, k+j}^j F(x, \zeta_1, \dots, \zeta_j, 0, \dots, 0)|^p d\zeta_{1 \dots j} \\ &= h^j \int_{B_1^j[0]} |\partial_{k+1, \dots, k+j}^j F(x, h\zeta_1, \dots, h\zeta_j, 0, \dots, 0)|^p d\zeta_{1 \dots j} \end{aligned}$$

The relative codimension of $B_h^j[0]$ in $B_h^\kappa[0]$ is now $\kappa - j$, and we apply the (integer) trace theorem to the expression on the right hand side with respect to $F(h \cdot)$. We thus define a value $\kappa_p(j)$ as

$$\begin{aligned} p > 1 : \kappa_p(\kappa) &= 0, \kappa_p(j) = \min\{n \in \mathbb{N} : n > (\kappa - j)/p\}, 1 \leq j < \kappa \\ p = 1 : \kappa_p(j) &= \kappa - j, 1 \leq j \leq \kappa \end{aligned}$$

Then we see by the integer trace theorem that for c independent of F and h and multi-indices α of the last κ variables it holds

$$\begin{aligned} & \int_{B_1^j[0]} |\partial_{k+1, \dots, k+j}^j F(x, h\zeta_1, \dots, h\zeta_j, 0, \dots, 0)|^p d\zeta_{1 \dots j} \\ & \leq c \sum_{|\alpha|=0}^{\kappa_p(j)} \int_{B_1^\kappa[0]} h^{|\alpha|p} \|\partial_z^\alpha \partial_{k+1, \dots, k+j}^j F(x, h\zeta_1, \dots, h\zeta_\kappa)\|_p^p d\zeta. \end{aligned}$$

Rescaling onto $B_h^j[0] =]-h, h[^j$ on the left and $B_h^\kappa[0]$ on the right gives a division by h^j and h^κ on the left and right, respectively, and therefore

$$\begin{aligned} & \int_{B_h^j[0]} |\partial_{k+1, \dots, k+j}^j F(x, \zeta_1, \dots, \zeta_j, 0, \dots, 0)|^p d\zeta_{1 \dots j} \\ & \leq c \sum_{|\alpha|=0}^{\kappa_p(j)} \int_{B_h^\kappa[0]} h^{|\alpha|p - (\kappa - j)} \|\partial_z^\alpha \partial_{k+1, \dots, k+j}^j F(x, \zeta_1, \dots, \zeta_\kappa)\|_p^p d\zeta. \end{aligned}$$

We proceed by applying Fubini's theorem, thereby obtaining by $\frac{p}{p^*} = p - 1$ that

$$\begin{aligned} & \int_{\substack{x \in \omega \\ z \in B_h^\kappa[0]}} |z_1 \cdot \dots \cdot z_j|^{\frac{p}{p^*}} \sum_{|\alpha|=0}^{\kappa_p(j)} \int_{B_h^\kappa[0]} h^{|\alpha|p - (\kappa - j)} \|\partial_z^\alpha \partial_{k+1, \dots, k+j}^j F(x, \zeta_1, \dots, \zeta_\kappa)\|_p^p d\zeta \\ & \leq c h^{jp + (\kappa - j)} \int_{x \in \omega} \sum_{|\alpha|=0}^{\kappa_p(j)} \int_{B_h^\kappa[0]} h^{|\alpha|p - (\kappa - j)} \|\partial_z^\alpha \partial_{k+1, \dots, k+j}^j F(x, \zeta_1, \dots, \zeta_\kappa)\|_p^p d\zeta \\ & = c \int_{x \in \omega} \sum_{|\alpha|=0}^{\kappa_p(j)} \int_{B_h^\kappa[0]} h^{p(|\alpha| + j)} \|\partial_z^\alpha \partial_{k+1, \dots, k+j}^j F(x, \zeta_1, \dots, \zeta_\kappa)\|_p^p d\zeta. \end{aligned}$$

This last expression contains no derivatives of order less than j , and only some of those at least of order j . Now we have to see that $j \geq 1$ and consequently for $\kappa^*(j) = \kappa_p(j) + j \leq \kappa$ it holds that

$$\int_{x \in \omega} \sum_{|\alpha|=0}^{\kappa_p(j)} \int_{B_h^\kappa[0]} h^{p(|\alpha| + j)} \|\partial_z^\alpha \partial_{k+1, \dots, k+j}^j F(x, \zeta_1, \dots, \zeta_\kappa)\|_p^p d\zeta$$

$$\leq c \int_{x \in \omega} \sum_{|\beta|=j}^{\kappa_p^*(j)} h^{p \cdot |\beta|} \int_{B_h^k[0]} \|\partial_z^\beta F(x, \zeta_1, \dots, \zeta_k)\|_p^p d\zeta.$$

Because we will always face that for $j = 1$ derivatives of order 1 appear, and for $j = \kappa$ derivatives of order κ appear, we will loose nothing if we bound the latter by

$$\int_{x \in \omega} \sum_{|\beta|=j}^{\kappa_p^*(j)} h^{p \cdot |\beta|} \int_{B_h^k[0]} \|\partial_z^\beta F(x, \zeta_1, \dots, \zeta_k)\|_p^p d\zeta \leq c \int_{x \in \omega} \sum_{|\beta|=1}^{\kappa} h^{p \cdot |\beta|} \int_{B_h^k[0]} \|\partial_z^\beta F(x, \zeta_1, \dots, \zeta_k)\|_p^p d\zeta.$$

Taking all necessary sums and changing variable orders were necessary gives the ultimate goal in the form

$$\int_{\substack{x \in \omega \\ z \in B_h^k[0]}} |F(x, z)|^p \leq c \sum_{|\alpha|=1}^{\kappa} h^{p \cdot |\alpha|} \int_{\substack{x \in \omega \\ z \in B_h^k[0]}} \|\partial_z^\alpha F(x, z)\|_p^p.$$

□

9.24 Theorem — Leafwise Polynomial Friedrichs' Inequality —

Let $\omega \in \text{Lip}_k$ and let $\Omega_h = \omega \times B_h^k[0]$. Let $F \in W_p^1(\Omega_h)$ for some $1 \leq p < \infty$ be a continuous function that vanishes on ω . Let further the restriction of F to any $\{x\} \times B_h^k[0]$ be a polynomial of maximal degree $n \in \mathbb{N}$. Then we have the relation

$$\|F\|_{L_p(\Omega_h)}^p \leq c h^p \sum_{\substack{|\alpha|=1 \\ \alpha_1 = \dots = \alpha_k = 0}} \|\partial^\alpha F\|_{L_p(\Omega_h)}^p$$

for a constant $c = c(n) > 0$ independent of F and h .

Proof: We make the same assumptions as in the previous proof. Further, we define $P_x(z) = F(x, z)|_{\{x\} \times B_h^k[0]}$, and we notice that this is a polynomial of fixed degree for any $x \in \omega$ by assumption. Then we obtain by Fubini's theorem

$$\int_{\omega \times B_h^k[0]} |F|^p = \int_{\omega} \int_{B_h^k[0]} |P_x(\zeta)|^p.$$

Consequently, we just need to bound $\int |P_x(\zeta)|^p$ appropriately and reinsert the bound. Let us therefore suppose that P_x is in Taylor form w.r.t. variable z and Taylor expansion center x , so $z_0 = 0$. Then because $P_x(0) = 0$ by hypothesis, we have for suitable coefficients

$$P_x(z) = \sum_{0 \leq |\beta| \leq n} c_{\beta, x} z^\beta = \sum_{1 \leq |\beta| \leq n} c_{\beta, x} z^\beta,$$

where in particular $|\beta| > 0$ because $P_x(0) = 0$. Then we have that for an arbitrary multi-index $\alpha \leq \beta$ with $|\alpha| = 1$

$$(\partial_z^\alpha P_x)(z) = \sum_{\substack{\alpha \leq \beta \\ |\beta| \leq n}} \frac{c_{\beta, x}}{\langle \beta, \alpha \rangle} z^{\beta - \alpha}.$$

Now we transform $B_h^k[0]$ to $B_1^k[0]$ and see

$$\begin{aligned} \int_{B_h^k[0]} |P_x(\zeta)|^p d\zeta &= h^k \int_{B_1^k[0]} |P_x(h\zeta)|^p d\zeta \\ \int_{B_h^k[0]} |(\partial_z^\alpha P_x)(\zeta)|^p d\zeta &= h^k \int_{B_1^k[0]} |(\partial_z^\alpha P_x)(h\zeta)|^p d\zeta. \end{aligned}$$

So it suffices to prove that

$$\int_{B_1^k[0]} |P_x(h\zeta)|^p d\zeta \leq c h^p \sum_{|\alpha|=1} \int_{B_1^k[0]} |(\partial_z^\alpha P_x)(h\zeta)|^p d\zeta.$$

To see this, we apply the triangle inequality and Jensen's inequality to conclude that if $\|z\|_\infty \leq 1$

$$\begin{aligned} |P_x(hz)|^p &= \left| \sum_{1 \leq |\beta| \leq n} c_{\beta, x} (hz)^\beta \right|^p \leq c \sum_{1 \leq |\beta| \leq n} h^{p|\beta|} |c_{\beta, x} z^\beta|^p \\ &= c \sum_{1 \leq |\beta| \leq n} \sum_{\substack{|\alpha|=1 \\ \alpha \leq \beta}} |\langle \beta, \alpha \rangle|^p h^{p|\beta|} \left| \frac{c_{\beta, x}}{\langle \beta, \alpha \rangle} z^\beta \right|^p \\ &\leq c \sum_{1 \leq |\beta| \leq n} \sum_{\substack{|\alpha|=1 \\ \alpha \leq \beta}} h^{p|\beta|} \left| \frac{c_{\beta, x}}{\langle \beta, \alpha \rangle} z^\beta \right|^p \leq c \sum_{|\alpha|=1} h^{p|\beta|} \sum_{\substack{\alpha \leq \beta \\ |\beta| \leq n}} \left| \frac{c_{\beta, x}}{\langle \alpha, \beta \rangle} z^{\beta - \alpha} \right|^p |z^\alpha|^p. \end{aligned}$$

In particular $|z^\alpha|^p \leq 1$, and so we can deduce that

$$|P_x(hz)|^p \leq c \sum_{|\alpha|=1} h^{p|\beta|} \sum_{\substack{\alpha \leq \beta \\ |\beta| \leq n}} \left| \frac{c_{\beta, x}}{\langle \alpha, \beta \rangle} z^{\beta - \alpha} \right|^p.$$

Further, the expression

$$\left(\int_{B_1^k[0]} \sum_{\substack{\alpha \leq \beta \\ |\beta| \leq n}} |c_\beta z^{\beta - \alpha}|^p \right)^{\frac{1}{p}}$$

defines a norm on the finite dimensional space of polynomials spanned by the set

$$\{z \mapsto z^{\beta - \alpha} : \alpha \leq \beta, |\beta| \leq n\}.$$

This norm is hence equivalent to the standard $L_p(B_1^k[0])$ -norm because the dimension is finite. Moreover, there are only finitely many of those spaces that can appear, so an overall constant can be chosen. Additionally, the real numbers

$$\left\{ \frac{c_{\beta, x}}{\langle \alpha, \beta \rangle} h^{|\beta| - 1} : \alpha \leq \beta, |\beta| \leq n \right\}$$

are valid coefficients for the functions

$$\{z \mapsto z^{\beta-\alpha} : \alpha \leq \beta, |\beta| \leq n\}.$$

We can thus conclude by

$$\sum_{|\alpha|=1} h^{p|\beta|} \int_{B_1^K[0]} \sum_{\substack{\alpha \leq \beta \\ |\beta| \leq n}} \left| \frac{c_{\beta,x}}{\langle \alpha, \beta \rangle} \zeta^{\beta-\alpha} \right|^p d\zeta = \sum_{|\alpha|=1} h^p \int_{B_1^K[0]} \sum_{\substack{\alpha \leq \beta \\ |\beta| \leq n}} \left| \frac{c_{\beta,x}}{\langle \alpha, \beta \rangle} (h\zeta)^{\beta-\alpha} \right|^p d\zeta$$

that indeed

$$\int_{B_1^K[0]} |P_x(h\zeta)|^p d\zeta \leq c h^p \sum_{|\alpha|=1} \|\partial^\alpha P_x(h\cdot)\|_{L_p(B_1^K[0])}^p,$$

which finishes the proof. \square

9.3 Notes on Riemannian Geometry

In this section, we give a small revision of general concepts of Riemannian geometry that invoke our concepts of tangential calculus as special cases. We will be brief and sloppy, just to give a short justification of what we did for a reader unfamiliar with Riemannian geometry. The purpose is to give the reader a short glimpse at the “world behind” and why for example we do not need to care about differences of our definitions of concepts like gradient, Laplacian and Hessian from those in terms of — for example — parameterisations the reader might have encountered elsewhere. In our notation, we are a little more “analytic” than it is usual, but this seems appropriate in preparing the ground for a reader that is unfamiliar with geometry and more familiar with analysis.

Our concept of ESMs can be seen as special cases of the general concept of a Riemannian manifold $(M, g(\cdot, \cdot))$. There, $g(\cdot, \cdot)$ is the so-called *Riemannian metric* that essentially characterises the manifold as such. It is a symmetric, positive definite pointwise bilinear form on the pointwise tangent space $T_x M$, and depends smoothly on the point x , so we have $g_x(\cdot, \cdot)$ varying with $x \in M$. A special case is of course the Euclidean scalar product on the manifold \mathbb{R}^d , and another example is the *first fundamental form* in classical differential geometry, which precisely defines such a metric for the parameterised representation of a surface. Given this metric, concepts like orthonormal basis, derivative, gradient, covariant derivative, divergence etc. can be reasonably defined for the manifold setting when the manifold is *smooth*. For instance, a $g(\cdot, \cdot)$ -orthonormal basis τ^1, \dots, τ^k of $T_x M$ will vary

with $x \in M$ just as $g(\cdot, \cdot)$ does. One can then define the (Riemannian) gradient of a smooth function $f : M \rightarrow \mathbb{R}$ (sloppily) as

$$\nabla_M f = (D_{\tau^1} f, \dots, D_{\tau^k} f),$$

where for any τ^i one has in D_{τ^i} the directional derivative along $\tau^i(x)$ in x . This gives for a smooth tangent vector field v on M also the v -directional derivative as

$$\sum_{i=1}^k (D_{\tau^i} f) \cdot g(\tau^i, v).$$

The covariant derivative ∇_x of a tangent vector field v along a tangent vector field x can be obtained from $\nabla_{\tau^1} v, \dots, \nabla_{\tau^k} v$, where for any τ^i one has

$$\nabla_{\tau^i} v(x) = \Pi_{T_x M}((D_{\tau^i} v)(x)).$$

Then one gets suitable coefficient *functions* $\alpha_1, \dots, \alpha_k$ such that $v = \alpha_1 \tau^1 + \dots + \alpha_k \tau^k$ the relation

$$\nabla_x v = \sum_{i=1}^k \alpha_i \cdot \nabla_{\tau^i} v.$$

The coefficient functions are necessary because, in contrast to the Euclidean setting, the tangent space, and consequently the $g(\cdot, \cdot)$ -ONB, depend on the point. Following this, the (Riemannian) divergence appears as

$$\operatorname{div}_g v = \sum_{i=1}^k g(\nabla_{\tau^i} v, \tau^i)$$

and the Hessian for two tangent vector fields x, v with $x = \alpha_1 \tau^1 + \dots + \alpha_k \tau^k$ and $v = \beta_1 \tau^1 + \dots + \beta_k \tau^k$ appears as

$$H_f^M(x, v) = g(\nabla_x \nabla_M f, v) = \sum_{i=1}^k \alpha_i \cdot g(\nabla_{\tau^i} \nabla_M f, v) = \sum_{i,j=1}^k \alpha_i \cdot \beta_j \cdot g(\nabla_{\tau^i} \nabla_M f, \tau^j).$$

Thereby one can deduce a matrix representation $H_f^M = (h_{ij}^g)_{i,j=1}^k$ for the Riemannian Hessian, with entries

$$h_{ij}^g = g(\nabla_{\tau^i} \nabla_M f, \tau^j).$$

The Laplacian is then simultaneously obtained as the divergence of the gradient or the trace of the Hessian. Further concepts like *parallelism*, *curvature tensor* or *sectional curvature* appear in the same way as in our tangential calculus in the general setting, where one inserts the respective general Riemannian operations and the Riemannian metric instead of the Euclidean scalar product employed in the main part of this thesis.

In the situation of local coordinates (so parameterisations), one can explicitly express the respective concepts by suitable formulae in terms of the parameterisations and the matrix representation of the metric. Of course, all concepts introduced, such as derivative, gradient and divergence, are parameterisation invariants. Because of that, we can in fact always demand that they are given in normal coordinates, so with respect to the exponential map, whereby the formulae simplify significantly. In particular, for normal coordinates in a point $x \in M$, one obtains precisely the expressions we stated for these concepts in the main part in that single point⁽²⁾. Consequently, as the expressions coincide pointwise for each point and smooth functions, they do also as operators in the general case.

This last conclusion can also be drawn in a different way: In our case of embedded submanifolds, we are in a technically more comfortable situation. The metric of an ESM is induced by the ambient space, and can just be seen as the restriction of the metric of the ambient space — so just the Euclidean scalar product. The only thing that varies is the space it is defined on, namely the tangent space. This is precisely the metric representation of normal coordinates to a point $x \in M$ in that point. With this "induced" approach to the metric, one obtains the previously mentioned concepts and constructs as well just in the way we have introduced them in the main part of the thesis: The $g(\cdot, \cdot)$ -ONB is then just an arbitrary, but locally smooth choice of a Euclidean ONB τ^1, \dots, τ^k of the tangent space $T_x M$. The gradient is then easily seen to be the projection of the Euclidean gradient to the tangent space, and anything else follows then in the same way by insertion. And as anything is just determined by the metric, we do have the same object regardless what approach we take to the metric — be it induced by the ambient metric or be it by the parameterisations.

For a deeper insight, the reader is referred to, among others, the textbooks [7, 9, 34, 51, 73, 83]. For example, the introductory chapter of [9] gives a brief but quite comprehensive introduction into the matter.

⁽²⁾This is a direct consequence of properties of normal coordinates, namely that the representation matrix G of g and its inverse coincide with the unit matrix in that point and that any partial derivative of that matrix G vanishes in that point, cf. [9, Prop. 1.25].

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